1
Gas phase Energy: -1284.39082626681 hartrees
Solvation Energy: -0.01299837360 hartrees
Zero Point Energy: 258.858 kcal/mol
Free Energy: -27.641 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.2033845924	-0.0255909078	0.1373000963
C2	0.0630221150	0.0828932431	3.6722449581
C3	2.2616944253	0.0778745543	2.5801253095
C4	1.8856852251	-1.2248869836	1.8486004039
N5	0.4147952970	-1.4449580526	1.6787587426
C6	-0.3189373895	-1.2426256108	2.9762331386
C7	-1.8232552624	-1.4599404716	2.7722476701
C8	-2.1038609033	-2.8905672780	2.2876892606
C9	-1.2759096191	-3.2059677627	1.0340726870
C10	0.2005680283	-2.8567932791	1.2258160861
C11	1.5712614187	0.0714809128	3.9526842990
C12	-0.2932534340	1.3906679790	2.9404700844
N13	0.4716073875	1.6033759893	1.6862390241
C14	1.9518406659	1.3937407089	1.8224996870
C15	2.7010434998	2.5888869183	2.4629501534
C16	0.8417800581	4.1244069325	1.7806905700
C17	2.3611885119	3.9226372920	1.7854994876
C18	0.1637218453	2.9360816745	1.0889589432
H19	-0.4935467975	0.0932544100	4.6181424744
H20	3.3511656843	0.0414471396	2.7066644330
H21	2.3364213241	-1.2651288930	0.8530664958
H22	2.2990048838	-2.0625158280	2.4362274154
H23	0.0338561816	-2.0387149365	3.6586035012
H24	-2.3356976712	-1.2698393157	3.7233823206
H25	-2.2024639543	-0.7363009021	2.0407100846
H26	-1.8505544458	-3.5987911839	3.0893972866
H27	-3.1712418050	-3.0210792957	2.0790974221
H28	-1.3454146374	-4.2706801243	0.7809743162
H29	-1.6631593413	-2.6410315910	0.1803545479
H30	0.7527278307	-2.9865160484	0.2919114217
H31	0.6463030527	-3.5255586125	1.9823530372
H32	1.8632776642	0.9351199015	4.5577470520
H33	1.8552343778	-0.8238884581	4.5192370683
H34	-0.1258788508	2.2140482492	3.6529935411
H35	-1.3539265857	1.4145067338	2.6725982345
H36	2.3188282800	1.2969410270	0.7918820674
H37	3.7776977591	2.3865650132	2.3997759171
H38	2.4627217723	2.6660086244	3.5308715041

H39	0.5690974325	5.0376576666	1.2389857267
H40	0.4775116155	4.2526922343	2.8092778517
H41	2.7288542887	3.9170090983	0.7500104197
H42	2.8703202503	4.7472010960	2.2977441792
H43	-0.9244016334	3.0407530075	1.0736091234
H44	0.4735501154	2.8977870410	0.0415667342
H45	-0.5579154718	-1.1130752700	-0.8657507625
Cl46	-0.8129167274	1.3624866126	-1.6609628254

2
Gas phase Energy: -1458.87429835517 hartrees
Solvation Energy: -0.01516780078 hartrees
Zero Point Energy: 334.585 kcal/mol
Free Energy: -33.738 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.8634714586	-0.7610844408	1.3344359410
C2	0.8547266394	0.9301346846	3.9342299842
C3	2.3976699963	0.0277735003	2.2516933615
C4	1.7996469848	-1.3751949570	2.4684867735
N5	0.4005786865	-1.3846910992	3.0039996804
C6	0.2694768871	-0.4756970974	4.1955156936
C7	-1.1710917408	-0.4934783590	4.7198347507
C8	-1.5700156063	-1.9100899845	5.1606999876
C9	-1.3324842056	-2.9138188475	4.0238109837
C10	0.0724514073	-2.7823692920	3.4333691647
C11	2.3420164610	0.7839121482	3.5880232045
C12	0.1757221155	1.7846330600	2.8469211161
N13	0.3420397965	1.2494240170	1.4720654876
C14	1.7519591956	0.8708113958	1.1235452308
C15	2.6528344171	2.0736614123	0.7481724835
C16	0.6202304661	3.4134197962	0.1534679072
C17	2.0118138841	2.9743218938	-0.3154201197
C18	-0.2369853967	2.1795548069	0.4588984440
H19	0.7422910952	1.4794503414	4.8777382475
H20	3.4415146822	-0.1390690351	1.9569868191
H21	1.7945904461	-1.9521472990	1.5396215497
H22	2.4511090751	-1.9027536255	3.1859165925
H23	0.9075098380	-0.9105328671	4.9877096909
H24	-1.2448212832	0.2051892861	5.5623695246
H25	-1.8516120937	-0.1404759859	3.9357009111
H26	-0.9741677786	-2.1949638108	6.0394379639
H27	-2.6198663754	-1.9321456764	5.4723262049
H28	-1.4577063641	-3.9425514672	4.3822867035
H29	-2.0657035360	-2.7537686797	3.2271306242

H30	0.1860258815	-3.4270495055	2.5585511016
H31	0.8213805842	-3.0891753632	4.1836770296
H32	2.8261607249	1.7628669063	3.5210797697
H33	2.8696990483	0.2212548537	4.3679720995
H34	0.5915657524	2.8013298976	2.9309609557
H35	-0.9004821851	1.8667613516	3.0270143400
H36	1.6617049709	0.2420969384	0.2275289263
H37	3.6131245382	1.6790226551	0.3929487706
H38	2.8760713433	2.6800545404	1.6345338841
H39	0.1126249955	4.0007131305	-0.6206463439
H40	0.7099708144	4.0678048454	1.0314160083
H41	1.9179277139	2.4225757920	-1.2609889772
H42	2.6550416061	3.8389426907	-0.5158960176
H43	-1.2371357529	2.4540539008	0.8045639523
H44	-0.3868560829	1.6030683466	-0.4575875134
H45	-1.5688588483	-2.1049798299	1.2352200663
Cl46	-2.2311217424	-0.2848082965	-0.5198841706
N47	-6.5184755091	-0.0672566128	-5.1075953870
C48	-7.2783432753	-1.1419700840	-4.4858371275
C49	-6.0110513463	0.8692109653	-4.1128207714
C50	-5.4463024162	-0.5882111483	-5.9432826201
H51	-6.6737755163	-1.7669107063	-3.7988220036
H52	-8.1118314779	-0.7227887109	-3.9116360558
H53	-7.6951531941	-1.7975303468	-5.2585246029
H54	-5.3076030676	0.4070947364	-3.3923109650
H55	-5.4894257583	1.6928246836	-4.6121767681
H56	-6.8457110505	1.2926021031	-3.5435616402
H57	-4.6890243842	-1.1661714251	-5.3770952000
H58	-5.8631899215	-1.2445141632	-6.7154280870
H59	-4.9309444734	0.2388681665	-6.4440254686

3
Gas phase Energy: -1458.85392866544 hartrees
Solvation Energy: -0.01306576102 hartrees
Zero Point Energy: 336.136 kcal/mol
Free Energy: -34.378 kcal/mol
final geometry:

	angstroms		
atom	x	y	z
Pd1	-1.7156679700	0.5780433232	0.2691720431
C2	0.7519474478	-0.4598369658	3.1130895825
C3	1.9690751925	0.4325915973	1.1804281358
C4	1.2196368886	-0.5489188852	0.2576150739
N5	-0.0999575940	-1.0161537579	0.7609592157
C6	-0.0157658673	-1.4428977424	2.1973560139
C7	-1.4154540289	-1.8234584679	2.6944086288

C8	-1.9697245133	-3.0070778019	1.8858778755
C9	-1.9052762362	-2.7073020192	0.3809039491
C10	-0.5225316496	-2.1981473331	-0.0362705818
C11	2.1595807985	-0.2461785035	2.5441212480
C12	0.1220613453	0.9203055066	3.3665027408
N13	0.0930360101	1.7495133521	2.1695435796
C14	1.3129924363	1.8235800306	1.3535321771
C15	2.3261866598	2.8774843970	1.8730052496
C16	0.3998625728	4.1233361087	2.9383904580
C17	1.6549052365	4.2485352526	2.0609814018
C18	-0.5417813022	3.0565656422	2.3507659933
H19	0.8176138366	-0.9619398910	4.0878243380
H20	2.9452384419	0.5975934397	0.7045208641
H21	1.0508276780	-0.1048008140	-0.7276451494
H22	1.8858862264	-1.4235603525	0.1198552375
H23	0.5968299134	-2.3680970723	2.2167712362
H24	-1.3629968113	-2.0797066999	3.7605444276
H25	-2.0758665519	-0.9543771870	2.5817586343
H26	-1.3786180415	-3.9068221751	2.1104876967
H27	-3.0015436661	-3.2268322488	2.1843628835
H28	-2.1468409129	-3.6041723584	-0.2051659533
H29	-2.6339750204	-1.9237497274	0.1334045691
H30	-0.5274972083	-1.9020734293	-1.0897002232
H31	0.2266908887	-3.0064760846	0.0822540757
H32	2.7610093106	0.3702723252	3.2216392927
H33	2.6862717253	-1.2022920369	2.4259673340
H34	0.6852462368	1.3740015677	4.2089775570
H35	-0.9126366970	0.8117306415	3.7132049059
H36	0.9780041821	2.1611995984	0.3590250295
H37	3.1646428547	2.9573141013	1.1674945879
H38	2.7529648572	2.5523833498	2.8313816282
H39	-0.1243959361	5.0852773298	3.0043543246
H40	0.6903864567	3.8518133825	3.9631674421
H41	1.3636951381	4.6453410609	1.0770265263
H42	2.3654995776	4.9662099386	2.4895783158
H43	-1.4302343688	2.9219210650	2.9765920036
H44	-0.9076979020	3.3888560794	1.3702460953
Cl45	-3.4304400079	2.3025632709	-0.1766598046
H46	-3.2333760996	1.8262006850	-1.9467910435
N47	-3.0408560948	1.4727602455	-2.9640059999
C48	-3.8865554611	2.2614150522	-3.8928799531
C49	-1.5820348999	1.6816803403	-3.1777835516
C50	-3.3848138252	0.0235425832	-2.9413710727
H51	-3.6309467460	3.3175947293	-3.7918937481
H52	-3.7191893027	1.9344894557	-4.9225266248
H53	-4.9341281455	2.1186144813	-3.6227191726

H54	-1.0707432161	1.2041940611	-2.3308951271
H55	-1.2833174753	1.2479460260	-4.1364041865
H56	-1.3762411902	2.7533289060	-3.1652228424
H57	-4.4560378297	-0.0792289426	-2.7607898787
H58	-3.1126524787	-0.4352702003	-3.8964510779
H59	-2.8321131669	-0.4123892144	-2.0984155417

4_{trip}

Gas phase Energy: -1609.20980177534 hartrees
Solvation Energy: -0.01554037683 hartrees
Zero Point Energy: 341.158 kcal/mol
Free Energy: -35.146 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-1.4015671671	0.7815323012	1.2969160149
C2	1.6055035653	-0.6661711949	2.9645381524
C3	1.9154062759	-0.3257815890	0.5577481279
C4	0.6944538899	-1.2275356465	0.2855259950
N5	-0.2704953268	-1.3232620362	1.4086440377
C6	0.4048927647	-1.6025695569	2.7064781150
C7	-0.6248759696	-1.6349705359	3.8421990887
C8	-1.6531549674	-2.7469952991	3.5982865962
C9	-2.3003758371	-2.5644350288	2.2207761580
C10	-1.2561121369	-2.3961881374	1.1137727609
C11	2.6144805501	-0.8407152147	1.8243343419
C12	1.3010493115	0.8341748630	3.1364215710
N13	0.8254791240	1.5052711960	1.9037024807
C14	1.6310090572	1.1930522056	0.6785749438
C15	2.9479171899	2.0046114040	0.5672416090
C16	2.0071688045	3.7580854675	2.0899739062
C17	2.7295339190	3.5105824124	0.7611397076
C18	0.6883638580	2.9734489655	2.1093244796
H19	2.0498905555	-1.0007220648	3.9112065907
H20	2.5753638684	-0.4469230034	-0.3110200065
H21	0.1403822023	-0.8807552170	-0.5926494504
H22	1.0849759199	-2.2365751028	0.0502839745
H23	0.8432889003	-2.6204090313	2.6435233474
H24	-0.0996702781	-1.7904032990	4.7933456160
H25	-1.1340107508	-0.6642302075	3.8956004974
H26	-1.1474865525	-3.7221818282	3.6548590667
H27	-2.4183989245	-2.7445633668	4.3834841467
H28	-2.9268702193	-3.4292273985	1.9693467549
H29	-2.9576271185	-1.6898698569	2.2202311700
H30	-1.7536211267	-2.1373082480	0.1755265163
H31	-0.7085626202	-3.3469810284	0.9630821685

H32	3.5410769406	-0.2955728686	2.0311175970
H33	2.8857218082	-1.8973598773	1.7071793414
H34	2.2235190056	1.3046570019	3.5173928464
H35	0.5317713344	0.9893287358	3.8995139421
H36	0.9939906471	1.4948542728	-0.1636150352
H37	3.3886698784	1.8027123675	-0.4173297188
H38	3.6774359897	1.6582695276	1.3095353270
H39	1.7796383667	4.8227040653	2.2215735079
H40	2.6566975067	3.4711206104	2.9282927475
H41	2.1169278875	3.9055458594	-0.0613011815
H42	3.6888212002	4.0405765460	0.7243497738
H43	0.1449582634	3.1212172769	3.0471120511
H44	0.0354537570	3.3527372513	1.3190086106
H45	-4.4324407551	2.6619047135	1.0580709035
Cl46	-2.5823735765	3.1937968343	1.0757335750
N47	-5.4948666466	2.5646697192	1.2014824346
C48	-6.0677738615	1.8258317525	0.0360911541
C49	-5.6652082322	1.8121677854	2.4803469428
C50	-6.0107809614	3.9564249734	1.2951950679
H51	-5.7900109868	2.3563090523	-0.8759390021
H52	-5.6396644758	0.8191758275	0.0369737930
H53	-7.1565406494	1.7972501846	0.1366261022
H54	-5.2099841426	2.3944752403	3.2827934837
H55	-6.7318051056	1.6684851284	2.6738657624
H56	-5.1452937767	0.8576344646	2.3651650002
H57	-5.4775806455	4.4744554104	2.0935632609
H58	-5.8203257878	4.4669465862	0.3503315937
H59	-7.0838294920	3.9355266232	1.5029172401
O60	-3.1433485417	0.0321055876	0.2461042012
O61	-4.1998705816	-0.3913123135	0.9220556717

5_{trip}

Gas phase Energy: -1609.21465928912 hartrees
Solvation Energy: -0.01728268809 hartrees
Zero Point Energy: 340.545 kcal/mol
Free Energy: -37.005 kcal/mol
final geometry:

	angstroms		
atom	x	y	z
Pd1	-1.8034042035	0.2181019732	0.2802736111
C2	0.6091874188	1.6244796686	2.5078385600
C3	1.5465187022	-0.3570572969	1.3995992871
C4	0.3602111640	-1.1925321925	1.9193148848
N5	-0.8663279916	-0.4076106453	2.2291072190
C6	-0.5642435443	0.7920658785	3.0766265118
C7	-1.8460034770	1.5950546072	3.3359787799

C8	-2.9121423497	0.7277545784	4.0227502387
C9	-3.1541082942	-0.5667632657	3.2334175143
C10	-1.8363389437	-1.2861101121	2.9377053677
C11	1.8551629732	0.7313091243	2.4388929202
C12	0.4019463513	2.2915231466	1.1325141724
N13	0.2929870882	1.3162236901	0.0176265180
C14	1.3535461524	0.2677699609	-0.0047220321
C15	2.6970112332	0.7621661321	-0.5968958844
C16	1.4640998496	2.5471952949	-1.8701707961
C17	2.5076257779	1.4267724048	-1.9684688228
C18	0.1504300599	1.9943457084	-1.2972415156
H19	0.7725472109	2.4393775859	3.2244429769
H20	2.3912348042	-1.0539180820	1.3195850765
H21	0.0790509053	-1.9639499884	1.1949811586
H22	0.6990641222	-1.7086113279	2.8362748448
H23	-0.2087768628	0.4127237069	4.0555867937
H24	-1.5940966551	2.4566051619	3.9663420714
H25	-2.2336227811	1.9946897184	2.3911406178
H26	-2.5774421111	0.4753565330	5.0395189944
H27	-3.8462082216	1.2901716900	4.1295907158
H28	-3.8067543441	-1.2485506297	3.7926210054
H29	-3.6567140730	-0.3415983701	2.2843948854
H30	-2.0082035995	-2.1648977020	2.3082753578
H31	-1.3800571606	-1.6358744744	3.8823299705
H32	2.7400092872	1.3143845609	2.1637100399
H33	2.0650983687	0.2754185922	3.4147878399
H34	1.2540702452	2.9755781191	0.9805401622
H35	-0.5042981748	2.9042503844	1.1114537589
H36	0.9743692119	-0.5137286170	-0.6789982275
H37	3.3781787345	-0.0951210371	-0.6748569215
H38	3.1753615416	1.4792949321	0.0812354263
H39	1.2633828402	2.9830370389	-2.8564881448
H40	1.8462585259	3.3625687807	-1.2422285379
H41	2.1662123832	0.6759869052	-2.6960142536
H42	3.4655147502	1.8102261522	-2.3394766902
H43	-0.6017494025	2.7791984754	-1.1753488398
H44	-0.2580305964	1.2551016447	-1.9975116740
H45	-4.1080592934	3.8631840719	-0.9303272331
Cl46	-2.8260350419	4.3921964947	0.2779857047
N47	-4.9041074463	3.7004595642	-1.6746917245
C48	-5.8721029226	2.7222298147	-1.1037321760
C49	-5.5143392100	5.0395038138	-1.8781431685
C50	-4.2526312394	3.1840145647	-2.9103217468
H51	-5.3717112081	1.7601628590	-0.9722205717
H52	-6.2100969571	3.0995989015	-0.1372084329
H53	-6.7237277585	2.6169551471	-1.7825135938

H54	-5.9130951939	5.3903965518	-0.9255430796
H55	-4.7381776495	5.7301706955	-2.2104765287
H56	-6.3121450571	4.9742100028	-2.6231778134
H57	-3.7725418527	2.2323830400	-2.6701309878
H58	-5.0061526613	3.0515458709	-3.6923043167
H59	-3.5033505797	3.9096144038	-3.2322322274
O60	-4.0405929381	0.0039058104	-0.7362471243
O61	-3.0426771813	0.5865023923	-1.3777876510

5_{sing}

Gas phase Energy: -1609.23669180005 hartrees
Solvation Energy: -0.02041092768 hartrees
Zero Point Energy: 342.303 kcal/mol
Free Energy: -34.238 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-1.7020234263	0.3595617606	0.0530020488
C2	0.4744218587	1.6495459458	2.4676146840
C3	1.3565749986	-0.4099619008	1.4570984861
C4	0.0776790175	-1.1502315989	1.8944617111
N5	-1.1095318097	-0.2653559699	2.0769164445
C6	-0.7901720079	0.9072987629	2.9583839569
C7	-2.0211858593	1.8033761928	3.1393022466
C8	-3.2025366826	1.0127905978	3.7203603178
C9	-3.4882254789	-0.2338082609	2.8718267811
C10	-2.2201254854	-1.0646404440	2.6733920858
C11	1.6609786955	0.6761248566	2.5009313555
C12	0.3974201626	2.2963449361	1.0703376853
N13	0.2831893321	1.2981610048	-0.0379283314
C14	1.3069024287	0.1980473999	0.0330311064
C15	2.7102180401	0.6291499425	-0.4547775151
C16	1.6772468419	2.4516557071	-1.8381409237
C17	2.6638860465	1.2779548394	-1.8449725053
C18	0.2942149677	1.9774285969	-1.3749241698
H19	0.6404671006	2.4696777473	3.1770351210
H20	2.1550942132	-1.1631897856	1.4479658864
H21	-0.1986817437	-1.9205767625	1.1675243138
H22	0.2948362189	-1.6581695886	2.8502798538
H23	-0.5300667872	0.4935730254	3.9519484782
H24	-1.7478009117	2.6266618731	3.8102724734
H25	-2.3023578959	2.2623158296	2.1849125963
H26	-2.9700280905	0.7075129994	4.7513028749
H27	-4.0912216063	1.6512052838	3.7755312400
H28	-4.2445582387	-0.8681243127	3.3501789465
H29	-3.8777701690	0.0537332669	1.8886463912

H30	-2.4109459040	-1.9092729442	2.0049108244
H31	-1.8782177380	-1.4689661100	3.6427541921
H32	2.6004295792	1.1943528730	2.2843277533
H33	1.7692449989	0.2257593600	3.4954133537
H34	1.3074087159	2.9013515412	0.9423868993
H35	-0.4572323499	2.9731305769	0.9801777027
H36	0.9468865680	-0.5726183704	-0.6614483782
H37	3.3523281541	-0.2607251782	-0.4647227363
H38	3.1667058350	1.3336118504	0.2503442062
H39	1.5728603677	2.8827429696	-2.8408400231
H40	2.0518645671	3.2562899278	-1.1927085949
H41	2.3414074450	0.5350764408	-2.5885516007
H42	3.6664136713	1.6066315869	-2.1423550073
H43	-0.4211049796	2.8018893270	-1.3148258897
H44	-0.0969885868	1.2542865930	-2.0985739562
H45	-4.0022042220	3.7084757791	-0.5732169653
Cl46	-2.6191781011	4.5129535270	0.4020308173
N47	-4.8578294767	3.3989357129	-1.1707141039
C48	-5.5117369770	2.2492197064	-0.4807767977
C49	-5.7364868127	4.5953989938	-1.2314637336
C50	-4.3300076771	3.0137800542	-2.5109986719
H51	-4.8219904044	1.3970392132	-0.4532214224
H52	-5.7708365366	2.5634788343	0.5322359213
H53	-6.4206228227	1.9771031791	-1.0260482699
H54	-6.0271858806	4.8707851596	-0.2168381943
H55	-5.1757258929	5.4198457407	-1.6740443427
H56	-6.6220897074	4.3710782366	-1.8322991981
H57	-3.7108859073	2.1190779553	-2.3782920809
H58	-5.1689567800	2.8075890704	-3.1824926451
H59	-3.7367748058	3.8454329808	-2.8962640224
O60	-3.5007669104	-0.2397488277	-0.6490442682
O61	-2.7714253850	0.4282983183	-1.6474249085

6_{sing}

Gas phase Energy: -1609.22494321899 hartrees
Solvation Energy: -0.01663548347 hartrees
Zero Point Energy: 340.866 kcal/mol
Free Energy: -36.421 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-1.3334565203	-0.4715812588	0.9819881362
C2	1.5814097684	0.4115385940	2.5821634665
C3	2.0034048913	-0.4512722199	0.3164793355
C4	1.2722697407	-1.7548638908	0.6865805368
N5	0.2844440896	-1.6029272017	1.8047163485

C6	0.8904164412	-0.9098578718	2.9924210314
C7	-0.1355695846	-0.7797921926	4.1249042318
C8	-0.6636119325	-2.1564970226	4.5547629125
C9	-1.2243962847	-2.9153045452	3.3449154074
C10	-0.2149523518	-2.9616433170	2.1971058301
C11	2.6973099267	0.0881452033	1.5780146252
C12	0.6727010972	1.5054365822	1.9829795023
N13	0.0811370187	1.1221018090	0.6684730226
C14	1.1087643162	0.6350213195	-0.3288369021
C15	1.9471713418	1.7836672547	-0.9350567661
C16	0.0713379708	3.3983246906	-0.4844608520
C17	1.0767069198	2.8997094453	-1.5297673292
C18	-0.7468389290	2.2269194097	0.0708345803
H19	2.0104365505	0.8300797220	3.5013886144
H20	2.7502584192	-0.7283002108	-0.4373622977
H21	0.7301242895	-2.1621466007	-0.1713727338
H22	2.0270419100	-2.4963555490	0.9948144916
H23	1.6980626394	-1.5699212404	3.3572357921
H24	0.3464407397	-0.2702362516	4.9682545893
H25	-0.9712915700	-0.1501612366	3.7952612502
H26	0.1549770315	-2.7316307512	5.0104380134
H27	-1.4349670633	-2.0433673864	5.3240508566
H28	-1.4737437350	-3.9476790019	3.6162630921
H29	-2.1479391356	-2.4435829831	2.9938922104
H30	-0.6602494571	-3.4115882236	1.3061525287
H31	0.6604620947	-3.5665888324	2.4857455291
H32	3.2991324086	0.9753685934	1.3616511561
H33	3.3801672537	-0.6643398352	1.9909564010
H34	1.2768231275	2.4169323541	1.8788982365
H35	-0.1582911171	1.7457706847	2.6525500270
H36	0.5170268189	0.1855002871	-1.1358669056
H37	2.5865774656	1.3487046034	-1.7126234412
H38	2.6214279401	2.2104301521	-0.1821555330
H39	-0.6299235996	4.1138821218	-0.9289649187
H40	0.5877486727	3.9332511335	0.3248882703
H41	0.5547275152	2.5258581157	-2.4202671956
H42	1.7169424889	3.7237876145	-1.8660533278
H43	-1.4504280237	2.5544069842	0.8432359367
H44	-1.3210662865	1.7674909644	-0.7417713419
O45	-2.9579731010	-1.6080664431	0.9634530742
O46	-3.4075933108	-0.4151619867	0.3513171981
H47	-3.1845071091	-0.5447401617	-0.6548745625
Cl48	-2.1868803761	-0.4910710012	-2.2572564729
N49	0.2652614027	1.8206636352	-4.8586789669
C50	1.1076817781	2.6104977574	-5.7433899305
C51	0.5879574635	0.3992807294	-4.9406957345

C52	-1.1531493863	2.0499422559	-5.1239870413
H53	0.8781835827	3.6753212374	-5.6249923261
H54	2.1632423504	2.4596651383	-5.4895927789
H55	0.9782686435	2.3539588772	-6.8142509386
H56	-0.0472160623	-0.1590885824	-4.2469696870
H57	0.4414530789	-0.0167038852	-5.9573107617
H58	1.6381352737	0.2413298394	-4.6662728553
H59	-1.7554779710	1.4633998841	-4.4245508545
H60	-1.3874279030	3.1116109954	-4.9853253541
H61	-1.4441810957	1.7713024263	-6.1558627373

7_{sing}

Gas phase Energy: -1434.73697499909 hartrees
Solvation Energy: -0.01960954841 hartrees
Zero Point Energy: 264.658 kcal/mol
Free Energy: -30.004 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.5826521813	-0.2892443341	0.1203480749
C2	-0.0481764925	-0.1001810803	3.5201644818
C3	2.0537363475	-0.0697435241	2.2395772716
C4	1.6690207686	-1.4119660127	1.5922613902
N5	0.1921185469	-1.6677646523	1.5617982782
C6	-0.4352343691	-1.4688896604	2.9124843692
C7	-1.9425374882	-1.7466778992	2.8531595243
C8	-2.2256604338	-3.1743446829	2.3625361419
C9	-1.5325856114	-3.4255266889	1.0168849804
C10	-0.0475033669	-3.0670256511	1.0793421992
C11	1.4790653342	-0.0388801690	3.6645116966
C12	-0.5219182043	1.1508198327	2.7532506542
N13	0.1107378072	1.2890590924	1.4110283434
C14	1.6204017757	1.1822546584	1.4393031558
C15	2.3050577683	2.4653384923	1.9604144784
C16	0.3168978188	3.8275627153	1.2545191182
C17	1.8447682153	3.7149272529	1.1976009924
C18	-0.3214608895	2.5460557468	0.7073397732
H19	-0.5229412851	-0.0604558858	4.5086276073
H20	3.1497910048	-0.0544399230	2.2725991317
H21	2.0302785925	-1.4714413085	0.5619862660
H22	2.1462088572	-2.2215492449	2.1679361895
H23	0.0129348718	-2.2293350016	3.5772765790
H24	-2.3607645281	-1.5926755272	3.8553855424
H25	-2.4236417876	-1.0242779101	2.1821281840
H26	-1.8604217276	-3.8927803677	3.1100291692
H27	-3.3049573818	-3.3363984939	2.2715742897

H28	-1.6141801486	-4.4801601853	0.7296978416
H29	-2.0105228252	-2.8394957774	0.2249995991
H30	0.4148558961	-3.1513488002	0.0926848531
H31	0.4799135248	-3.7508279549	1.7647082660
H32	1.7839414567	0.8625527964	4.2043663810
H33	1.8465681305	-0.8943966897	4.2441664163
H34	-0.2940999904	2.0271494646	3.3758465336
H35	-1.6047705586	1.1397367550	2.5989098052
H36	1.9039193698	1.0567984892	0.3864923550
H37	3.3875457647	2.3280826762	1.8517481919
H38	2.1157496991	2.6069377023	3.0320575742
H39	-0.0364827688	4.6654183933	0.6430143605
H40	-0.0142187849	4.0298432636	2.2824098264
H41	2.1629829400	3.6433057419	0.1502822501
H42	2.3172173211	4.6088529626	1.6201200899
H43	-1.4142927803	2.5831747766	0.7582286581
H44	-0.0292595613	2.4209238162	-0.3413717949
O45	-1.2584447705	-1.3049828685	-1.4433530481
O46	-1.4329710422	0.0397349476	-1.8438386289
H47	-0.5228501758	0.3111181952	-2.2679922973
Cl48	1.2375473015	1.0177813122	-2.3510756572

8_{trip}
Gas phase Energy: -1434.72827238544 hartrees
Solvation Energy: -0.01042347256 hartrees
Zero Point Energy: 263.485 kcal/mol
Free Energy: -30.269 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.2753148254	-0.0221384222	0.1714346138
C2	0.1256762929	0.0527920271	3.7631360322
C3	2.2963312795	0.0352943632	2.6184711012
C4	1.9032935494	-1.2766497929	1.9133603039
N5	0.4369959723	-1.5018286380	1.7956037467
C6	-0.2698897732	-1.2839111480	3.0955023989
C7	-1.7798364803	-1.4868190553	2.9165724534
C8	-2.0824429846	-2.9116241904	2.4316727782
C9	-1.2864279454	-3.2194316535	1.1572733868
C10	0.2002621069	-2.8957530512	1.3253775767
C11	1.6396747759	0.0470725505	4.0070717936
C12	-0.2518842087	1.3503028859	3.0217644512
N13	0.4829553192	1.5521693950	1.7471589383
C14	1.9658700962	1.3398963628	1.8510205010
C15	2.7266341929	2.5446881071	2.4599484567
C16	0.8556376181	4.0744180474	1.7947191956

C17	2.3743393959	3.8698534418	1.7723188811
C18	0.1626809235	2.8761855823	1.1351763463
H19	-0.4077517083	0.0789563072	4.7220459852
H20	3.3886644442	0.0045369952	2.7192685142
H21	2.3226946396	-1.3199923999	0.9031161306
H22	2.3509957394	-2.1060371215	2.4904117793
H23	0.0809788694	-2.0704028432	3.7926748187
H24	-2.2773501957	-1.2914457981	3.8745911132
H25	-2.1640954086	-0.7586457487	2.1907122560
H26	-1.8109627503	-3.6263986880	3.2216134613
H27	-3.1556926166	-3.0355667927	2.2502337606
H28	-1.3791562500	-4.2775469659	0.8858118795
H29	-1.6844907076	-2.6408180503	0.3179662100
H30	0.7216569241	-3.0177956225	0.3723666896
H31	0.6554095014	-3.5925979141	2.0523914085
H32	1.9462109152	0.9174953099	4.5953107476
H33	1.9371144872	-0.8420166838	4.5764849025
H34	-0.0692436637	2.1837414627	3.7189969056
H35	-1.3188905746	1.3696816040	2.7800990739
H36	2.3101789594	1.2317201525	0.8138423856
H37	3.8017039282	2.3410155058	2.3784139794
H38	2.5091870949	2.6352654976	3.5310734795
H39	0.5724192088	4.9797230330	1.2453163406
H40	0.5108869668	4.2162447572	2.8279758798
H41	2.7218955644	3.8509653398	0.7299479859
H42	2.8941385121	4.7003114738	2.2637165797
H43	-0.9252269154	2.9817918694	1.1386400658
H44	0.4568122970	2.8231680008	0.0836450749
O45	-0.3911000360	-1.6152524800	-1.4169659299
O46	-0.7000673157	-1.2151297901	-2.6507666274
H47	-0.9340213225	-0.2289821354	-2.5285188563
Cl48	-1.2140977593	1.4762735324	-1.6527247110

8_{sing}

Gas phase Energy: -1434.75080300078 hartrees
Solvation Energy: -0.01491647831 hartrees
Zero Point Energy: 265.330 kcal/mol
Free Energy: -29.517 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.1434733715	-0.0062874231	0.1373342654
C2	-0.0107702751	0.0567179303	3.6519569024
C3	2.2094802545	0.0413398883	2.6034038911
C4	1.8462027841	-1.2698590513	1.8819736200
N5	0.3785795853	-1.4790827375	1.6842227402

C6	-0.3753567594	-1.2758085421	2.9673320934
C7	-1.8755603279	-1.5072181957	2.7554196544
C8	-2.1308340178	-2.9554934084	2.3177415828
C9	-1.3124033724	-3.2680418305	1.0602180713
C10	0.1621615871	-2.8878061772	1.2096185554
C11	1.4909390827	0.0538063293	3.9612658176
C12	-0.3639052835	1.3437404607	2.8876730136
N13	0.4292612122	1.5520335231	1.6415703769
C14	1.9158809290	1.3492392472	1.8259811268
C15	2.6411197720	2.5474529909	2.4878048029
C16	0.7895298907	4.0801861035	1.8056041218
C17	2.3088149565	3.8892696752	1.8263215054
C18	0.1372905871	2.9081948040	1.0670532427
H19	-0.5862057325	0.0838580293	4.5858735542
H20	3.2961161262	0.0089868617	2.7515231541
H21	2.3199369629	-1.3299368885	0.8978466542
H22	2.2408523862	-2.1016090421	2.4894457032
H23	-0.0240175449	-2.0637217883	3.6591422670
H24	-2.3979817884	-1.2849295034	3.6941624808
H25	-2.2549336470	-0.8149410773	1.9936263586
H26	-1.8520612822	-3.6328911596	3.1380063617
H27	-3.1969782328	-3.1157850981	2.1243323789
H28	-1.3544879889	-4.3388489398	0.8268891217
H29	-1.7251347269	-2.7362511809	0.2018892851
H30	0.6626968717	-2.9883824875	0.2455253366
H31	0.6550312586	-3.5513942342	1.9399159190
H32	1.7705581750	0.9231718415	4.5634954313
H33	1.7628683259	-0.8347243426	4.5434399367
H34	-0.2140725888	2.1864274644	3.5775620085
H35	-1.4174521846	1.3534333996	2.5942304823
H36	2.3104420082	1.2525403666	0.8066688372
H37	3.7183827218	2.3466905389	2.4377810676
H38	2.3883333570	2.6109484725	3.5526218441
H39	0.5152939776	5.0003595478	1.2769771780
H40	0.4073834484	4.1850888240	2.8299061206
H41	2.6904297886	3.9036972053	0.7963658102
H42	2.8066210176	4.7058742615	2.3612404035
H43	-0.9496924057	3.0058915690	1.0165294873
H44	0.4868973074	2.8966550976	0.0342830499
O45	-0.3909217066	-1.4533911444	-1.1791458874
O46	-1.7268917834	-1.4232483746	-1.6861585640
H47	-1.6870197230	-0.6258382239	-2.2496206314
Cl48	-0.6477046582	1.4941772608	-1.6922020467

9_{trip}

Gas phase Energy: -1609.21289600578 hartrees

Solvation Energy: -0.01156043685 hartrees
Zero Point Energy: 339.317 kcal/mol
Free Energy: -38.620 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.7062787809	0.5443505836	0.4579632290
C2	0.4913864828	-1.2042871897	3.3846420973
C3	1.2927198619	-2.2654094912	1.3221543312
C4	-0.1651956675	-2.4452845329	0.8589957620
N5	-1.1295122639	-1.4891133951	1.4665940033
C6	-0.9787198721	-1.4099695674	2.9528907597
C7	-1.9631645652	-0.3856864524	3.5317757911
C8	-3.4112015792	-0.7790135468	3.2069256522
C9	-3.5813298531	-0.9804699640	1.6958145997
C10	-2.5147854053	-1.9193098443	1.1263577994
C11	1.3250707209	-2.3768691661	2.8538789983
C12	1.1706317817	0.1148661101	2.9671518221
N13	1.3797257086	0.2468758957	1.5028615062
C14	1.9918475824	-0.9632432432	0.8575088097
C15	3.5260002031	-1.0627283818	1.0505401805
C16	3.6475633992	1.4111366008	1.4371079691
C17	4.2513820024	0.2328137311	0.6652943321
C18	2.1401274500	1.4878640795	1.1679671454
H19	0.4865449441	-1.2150132287	4.4821361554
H20	1.8537969592	-3.0945445094	0.8728042466
H21	-0.2466042568	-2.3452743672	-0.2280586832
H22	-0.4670841252	-3.4765591112	1.1171801200
H23	-1.2647928788	-2.3992004442	3.3617488112
H24	-1.8130111699	-0.3286308704	4.6169568022
H25	-1.7466906239	0.6071119922	3.1168031753
H26	-3.6590879410	-1.7101904802	3.7360913414
H27	-4.1070777170	-0.0152936388	3.5710358317
H28	-4.5675557498	-1.4012068597	1.4674486322
H29	-3.5200302941	-0.0169217862	1.1797959163
H30	-2.5918139599	-1.9592829053	0.0366315798
H31	-2.6698582424	-2.9421646784	1.5149373818
H32	2.3470385194	-2.3403059629	3.2435580853
H33	0.8964688451	-3.3340790356	3.1750611718
H34	2.1282837949	0.1694059385	3.5093403688
H35	0.5798165165	0.9798672216	3.2834045364
H36	1.8093659110	-0.8341227080	-0.2176643805
H37	3.8886377446	-1.9030766316	0.4454295837
H38	3.7674894380	-1.3048589268	2.0925268205
H39	4.1004831710	2.3593202988	1.1250914248
H40	3.8564638740	1.3042174529	2.5101106382

H41	4.1423195992	0.4123189180	-0.4133728467
H42	5.3252905312	0.1374451666	0.8625142724
H43	1.6704218847	2.3132560171	1.7087735862
H44	1.9731303664	1.6898658034	0.1066335513
O45	-2.4333487860	0.3649477318	-0.9727391637
O46	-2.5953996208	1.3572043230	-1.8515357375
H47	-1.9146732947	2.0542269702	-1.5488987415
Cl48	-0.4750718914	2.8724114761	-0.5288650627
N49	-0.5291241879	-0.1748698610	-5.8193699703
C50	-1.3846070564	-1.3498557988	-5.7553885815
C51	-1.2875305676	1.0492043692	-5.5901507782
C52	0.5947171733	-0.2834020310	-4.9013302974
H53	-1.8541937846	-1.4978343901	-4.7619787377
H54	-2.1884129063	-1.2653327743	-6.4950313658
H55	-0.8016665173	-2.2478108237	-5.9897323236
H56	-1.7472180109	1.0960016400	-4.5842706551
H57	-0.6301549528	1.9178528104	-5.7023527425
H58	-2.0887397089	1.1325022892	-6.3326758470
H59	0.2859856998	-0.3437770219	-3.8377575881
H60	1.1812901252	-1.1793176897	-5.1355537880
H61	1.2488259846	0.5886227537	-5.0089337204

9_{sing}

Gas phase Energy: -1609.23656591350 hartrees
Solvation Energy: -0.01448730840 hartrees
Zero Point Energy: 341.258 kcal/mol
Free Energy: -35.784 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.5217405944	0.0612305672	0.1722209691
C2	0.5792620985	-0.1181318880	3.5127630770
C3	2.4198921305	-0.0111051879	1.8914878332
C4	1.8747826133	-1.2772632543	1.2048579700
N5	0.4097015961	-1.5014249276	1.4032308274
C6	0.0373499097	-1.4037344467	2.8558752538
C7	-1.4646827546	-1.6435472362	3.0463584015
C8	-1.8403935913	-3.0572396659	2.5828338712
C9	-1.3963317727	-3.2616024652	1.1300739696
C10	0.0673694645	-2.8766803604	0.9056212812
C11	2.1084554466	-0.1105698816	3.3930400362
C12	0.0256420288	1.2122858438	2.9758963113
N13	0.4354411257	1.5225773733	1.5755313137
C14	1.9158414305	1.3400647840	1.3231075842
C15	2.7947346095	2.5058440539	1.8409225909
C16	0.8235497296	4.0410107478	1.8149596754

C17	2.2882489818	3.8825140123	1.3971755695
C18	-0.0075457222	2.9088782436	1.2050290366
H19	0.2857661430	-0.1715846892	4.5687751682
H20	3.5048131996	-0.0271179489	1.7287151668
H21	2.0591113836	-1.2594597112	0.1266820730
H22	2.4220978021	-2.1407356630	1.6190149815
H23	0.5624525445	-2.2338543931	3.3635568849
H24	-1.7073237170	-1.5028520319	4.1070477528
H25	-2.0351386826	-0.9002134376	2.4757300832
H26	-1.3545311262	-3.7922575769	3.2409190778
H27	-2.9202244559	-3.2165159251	2.6747949606
H28	-1.5111305700	-4.3113720036	0.8340666778
H29	-2.0205697666	-2.6699780879	0.4581924332
H30	0.2905947260	-2.9031998594	-0.1617549092
H31	0.7333041016	-3.5827947034	1.4295294905
H32	2.5435140225	0.7200599024	3.9565935567
H33	2.5327120744	-1.0321757602	3.8090343232
H34	0.3653158125	2.0074444077	3.6547627735
H35	-1.0677873649	1.2220464872	2.9930457700
H36	2.0099527043	1.3221927450	0.2299912293
H37	3.8150752371	2.3324133752	1.4772681823
H38	2.8504773866	2.4899064829	2.9357043569
H39	0.4105360394	4.9892145701	1.4519195644
H40	0.7430268223	4.0665623284	2.9099908019
H41	2.3666097166	3.9764250881	0.3054621967
H42	2.9144076392	4.6710071362	1.8296783275
H43	-1.0652880254	2.9862575452	1.4671273578
H44	0.0391415290	2.9766348313	0.1176500744
O45	-1.0543064125	-1.2936058565	-1.1642723093
O46	-2.4712028969	-1.3033430864	-1.3642341121
H47	-2.5955562117	-0.4494022259	-1.8236845907
Cl48	-1.5652567568	1.6695763977	-1.2965833043
N49	-1.6218477574	-1.5762871022	-5.7456249061
C50	-2.2632193143	-2.6472106383	-4.9915476755
C51	-2.5136552643	-0.4368403546	-5.9039240233
C52	-0.3636805255	-1.1808487240	-5.1220599785
H53	-2.5145516880	-2.3599738853	-3.9531041573
H54	-3.1849686788	-2.9545879730	-5.4982355200
H55	-1.5973419095	-3.5165228572	-4.9479827959
H56	-2.8097507859	0.0287726080	-4.9426776794
H57	-2.0275978512	0.3339236117	-6.5119813020
H58	-3.4273471182	-0.7501596982	-6.4216410933
H59	-0.4863323558	-0.8075961285	-4.0880471470
H60	0.3170635167	-2.0395019966	-5.0923454769
H61	0.1116882401	-0.3939067314	-5.7179528128

10_{sing}
Gas phase Energy: -1609.20857659934 hartrees
Solvation Energy: -0.01015941320 hartrees
Zero Point Energy: 342.325 kcal/mol
Free Energy: -33.649 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-1.7006402484	0.9001864952	1.3636478882
C2	1.3116268893	-0.6402656815	2.9847300535
C3	1.8972573576	0.0198653012	0.7012564687
C4	0.8943421613	-1.0203585701	0.1658654824
N5	-0.1419950244	-1.4194742958	1.1282551839
C6	0.3805872290	-1.7596918997	2.4617052174
C7	-0.7622765794	-2.1202602416	3.4235894444
C8	-1.6116054006	-3.2695805055	2.8629071405
C9	-2.1193971373	-2.9018470592	1.4629349353
C10	-0.9561026389	-2.5001666812	0.5533755167
C11	2.4907401871	-0.5093698154	2.0148735424
C12	0.6952202417	0.7585908413	3.2209688503
N13	0.3155879937	1.5339228607	1.9894988188
C14	1.3539320141	1.4593860328	0.8850327525
C15	2.5371378475	2.4438975012	1.0764991018
C16	1.1965698037	3.8690613659	2.6192893809
C17	2.1049925405	3.8796342643	1.3883687838
C18	-0.0076902937	2.9608718557	2.3476164441
H19	1.6683948151	-0.9686528611	3.9702053155
H20	2.6831081776	0.1010803852	-0.0605999488
H21	0.3870673870	-0.6307976210	-0.7229302632
H22	1.4872682697	-1.9039154476	-0.1499065264
H23	1.0308656898	-2.6612572385	2.3860202551
H24	-0.3269647754	-2.3998555424	4.3922786024
H25	-1.4092867859	-1.2509501896	3.5791478516
H26	-1.0054823067	-4.1860033222	2.8063511178
H27	-2.4505326715	-3.4857570037	3.5346875101
H28	-2.6515318128	-3.7457258122	1.0064945062
H29	-2.8266819620	-2.0681170862	1.5339522767
H30	-1.3333610895	-2.1515700073	-0.4140965948
H31	-0.3220356450	-3.3900982755	0.3543335457
H32	3.2681067412	0.1489771068	2.4163920010
H33	2.9575908355	-1.4879233270	1.8516154069
H34	1.4395557219	1.3390529669	3.7853523169
H35	-0.2018205497	0.6943157503	3.8418178249
H36	0.8141107475	1.7540085768	-0.0188067388
H37	3.1267515754	2.4139183780	0.1524110082
H38	3.2028884976	2.1023516242	1.8778111377

H39	0.8168150527	4.8724517006	2.8472626839
H40	1.7572208447	3.5391468928	3.5037073110
H41	1.5576626707	4.3025469836	0.5350400510
H42	2.9846634435	4.5134456245	1.5495082751
H43	-0.6878152552	2.9243195900	3.2035609632
H44	-0.5621374605	3.3721265899	1.4986076664
H45	-4.2317824095	1.2323033178	1.9762114901
Cl46	-1.5485688543	1.5232242116	-0.9704300430
N47	-5.1018308479	2.5106698085	1.8065799657
C48	-6.4020084350	2.2857205176	2.4554758335
C49	-4.3877916886	3.6370288627	2.4274167514
C50	-5.2553517336	2.7176866105	0.3542977092
H51	-6.8869519002	1.4131589326	2.0096249140
H52	-6.2516999798	2.0924892153	3.5212094047
H53	-7.0706138955	3.1541096912	2.3449177454
H54	-3.4114511924	3.7485378232	1.9500776324
H55	-4.9475143006	4.5804308379	2.3224748723
H56	-4.2350613695	3.4309177189	3.4898404777
H57	-4.2694797691	2.7893905636	-0.1122751124
H58	-5.7758244814	1.8601493503	-0.0803872720
H59	-5.8335418998	3.6289995246	0.1355910992
O60	-3.6650919636	0.3432074314	2.0271673387
O61	-2.7310910344	0.5668493273	3.0755635770

11
Gas phase Energy: -823.51230553835 hartrees
Solvation Energy: -0.00109352085 hartrees
Zero Point Energy: 251.007 kcal/mol
Free Energy: -27.134 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.4045933913	-0.0478902224	0.0476121018
C2	0.1733475896	0.0714160630	3.7563822600
C3	2.3569564662	0.0893649082	2.6372369003
C4	1.9921654389	-1.2222081831	1.9168574507
N5	0.5431878098	-1.4792831370	1.7956723109
C6	-0.2064142153	-1.2578196509	3.0581023625
C7	-1.7103742069	-1.4160831316	2.7907003812
C8	-2.0320471682	-2.8073527679	2.2242767377
C9	-1.1601312566	-3.0990342220	0.9953178497
C10	0.3177044928	-2.8513221224	1.3020228402
C11	1.6840680087	0.0754339069	4.0175848198
C12	-0.1978596403	1.3877688471	3.0423134537
N13	0.5460639495	1.6055338028	1.7912961337
C14	2.0125985982	1.3922237901	1.8737617831

C15	2.7804715921	2.6056362847	2.4615144038
C16	0.8966971572	4.1190943423	1.7497888777
C17	2.4176509311	3.9160747411	1.7461125076
C18	0.2126949037	2.8854406431	1.1355310363
H19	-0.3701124237	0.0741160733	4.7105881340
H20	3.4487215012	0.0758495284	2.7528148869
H21	2.4104393959	-1.2353316158	0.9046794416
H22	2.4760815339	-2.0439179276	2.4826929760
H23	0.0846395387	-2.0527237882	3.7784193566
H24	-2.2634434838	-1.2414358159	3.7228219020
H25	-2.0122237485	-0.6506539332	2.0604369652
H26	-1.8435680694	-3.5683564879	2.9950782008
H27	-3.0953385519	-2.8784200825	1.9667872133
H28	-1.2949579838	-4.1331370069	0.6538370884
H29	-1.4473852095	-2.4283647709	0.1695103228
H30	0.9204908692	-2.9854418908	0.3983987429
H31	0.6738519173	-3.5874846359	2.0515113848
H32	1.9740616283	0.9427165693	4.6206035322
H33	1.9851793166	-0.8189332793	4.5780245642
H34	-0.0372430700	2.1990602667	3.7782985269
H35	-1.2629136207	1.4028395754	2.7881189404
H36	2.3468018925	1.2732629579	0.8322511256
H37	3.8584124950	2.4137322503	2.3821273801
H38	2.5617852460	2.7136889494	3.5314756278
H39	0.6186850238	5.0123072622	1.1765106981
H40	0.5435789953	4.2827796270	2.7769741772
H41	2.7719388956	3.8751876496	0.7056292748
H42	2.9298802682	4.7630582141	2.2180026104
H43	-0.8773517580	2.9897490806	1.1414054047
H44	0.5200347896	2.8018056816	0.0846893975

12_{trip}

Gas phase Energy: -973.88381430488 hartrees

Solvation Energy: -0.00847004243 hartrees

Zero Point Energy: 255.058 kcal/mol

Free Energy: -29.893 kcal/mol

final geometry:

angstroms

atom	x	y	z
Pd1	-0.2517256887	-0.1272104334	0.1688671383
C2	0.1151041096	0.0470154973	3.7528919379
C3	2.3298832121	0.0409008163	2.6923308993
C4	1.9741750341	-1.2800483327	1.9845116861
N5	0.5174404297	-1.5218887982	1.8145700664
C6	-0.2424308167	-1.3019278932	3.0825287713
C7	-1.7423419053	-1.5146330302	2.8354158438

C8	-2.0218541847	-2.9307506215	2.3082152286
C9	-1.1580184563	-3.2303969718	1.0749069109
C10	0.3150944059	-2.9186940602	1.3448363353
C11	1.6193423874	0.0603946314	4.0540035763
C12	-0.2389423848	1.3384380399	2.9862983819
N13	0.5397048404	1.5158731596	1.7406743301
C14	2.0124923750	1.3275368859	1.8921943131
C15	2.7336920362	2.5611660219	2.4901343852
C16	0.8701474798	4.0363385821	1.6657380345
C17	2.3915657059	3.8508260391	1.7297832763
C18	0.2203133609	2.7897449360	1.0471318487
H19	-0.4542140392	0.0771735943	4.6909679425
H20	3.4178379218	0.0223363487	2.8362786938
H21	2.4286909411	-1.3237284186	0.9896766969
H22	2.4119878508	-2.1003655268	2.5831828747
H23	0.0826982675	-2.0789564380	3.8035535719
H24	-2.2829489365	-1.3412428645	3.7745244776
H25	-2.0941810003	-0.7747416527	2.1050735282
H26	-1.7989058961	-3.6613183593	3.0989136856
H27	-3.0845365220	-3.0437842156	2.0664504910
H28	-1.2468700199	-4.2847256378	0.7864456312
H29	-1.4954205102	-2.6294398402	0.2219376069
H30	0.9070650608	-3.0497010705	0.4340512980
H31	0.7136070439	-3.6154346929	2.1062012918
H32	1.8931509816	0.9422369903	4.6424063168
H33	1.9054863178	-0.8185910256	4.6448570938
H34	-0.0875773170	2.1773760509	3.6877176843
H35	-1.2966482731	1.3490105327	2.7051936964
H36	2.3912968135	1.1968628742	0.8686718310
H37	3.8151367458	2.3763176985	2.4650011653
H38	2.4649320095	2.6893055806	3.5460065376
H39	0.6067042459	4.9107805473	1.0587552978
H40	0.4726395086	4.2232666785	2.6723572941
H41	2.7912715970	3.7915416334	0.7073745089
H42	2.8739882956	4.7121742124	2.2060983892
H43	-0.8694383263	2.8804268794	1.0087068587
H44	0.5629135767	2.6854829381	0.0111127786
O45	-1.2086532371	-0.6229874549	-1.8947334159
O46	-1.0714236657	0.6545542238	-1.6398576430

12_{sing}
Gas phase Energy: -973.89424101039 hartrees
Solvation Energy: -0.01619321660 hartrees
Zero Point Energy: 256.471 kcal/mol
Free Energy: -27.508 kcal/mol
final geometry:

	angstroms		
atom	x	y	z
Pd1	-0.2103077321	-0.0697589391	0.2246248799
C2	0.0924179595	0.0336347262	3.7017979116
C3	2.3058010393	0.0229439410	2.6331165693
C4	1.9453503982	-1.2997967281	1.9310494587
N5	0.4835850830	-1.5136320886	1.7536549626
C6	-0.2703602207	-1.3145317587	3.0320811533
C7	-1.7741679618	-1.5275011736	2.8061020425
C8	-2.0611900211	-2.9266361388	2.2401133317
C9	-1.2303212404	-3.1725289885	0.9733270626
C10	0.2515838326	-2.8909674503	1.2282642062
C11	1.5981260358	0.0466596685	3.9963895091
C12	-0.2641117916	1.3210515002	2.9291251229
N13	0.5002091282	1.4804219861	1.6610705275
C14	1.9850218944	1.3072783610	1.8279336747
C15	2.6841878951	2.5472903392	2.4349925288
C16	0.8192027661	4.0119498018	1.6064420361
C17	2.3409609181	3.8366973248	1.6760022509
C18	0.1780563968	2.7700088372	0.9742878540
H19	-0.4738473221	0.0699600360	4.6413013532
H20	3.3941462216	0.0068694350	2.7731351495
H21	2.4038474358	-1.3552621606	0.9390328471
H22	2.3631061935	-2.1242927600	2.5362038432
H23	0.0692982980	-2.0969706513	3.7382856244
H24	-2.2919572266	-1.3846864373	3.7631097584
H25	-2.1489010945	-0.7690947581	2.1082978865
H26	-1.8155612919	-3.6832865347	2.9993625928
H27	-3.1295309684	-3.0335194090	2.0223249900
H28	-1.3313581864	-4.2123215729	0.6399891436
H29	-1.5805705337	-2.5299578087	0.1569691856
H30	0.8241341707	-2.9854176611	0.3012609854
H31	0.6582150176	-3.6176788705	1.9548487869
H32	1.8753667771	0.9279778704	4.5836060804
H33	1.8849489362	-0.8316412239	4.5874175374
H34	-0.0827142915	2.1684760511	3.6090149423
H35	-1.3246838116	1.3436768966	2.6642891931
H36	2.3701318784	1.1825724781	0.8077129293
H37	3.7664653700	2.3681123499	2.4189432296
H38	2.4066411280	2.6711290229	3.4887478306
H39	0.5514582023	4.8852053532	1.0000406708
H40	0.4153696825	4.1951575197	2.6111518656
H41	2.7467117487	3.7839355858	0.6560054958
H42	2.8151244910	4.6983374919	2.1597018353
H43	-0.9117026711	2.8502838184	0.9324723448
H44	0.5235477636	2.6696680535	-0.0597312458

O45	-0.9776874425	-0.8119875346	-1.4682251286
O46	-1.0127966474	0.5770147685	-1.4935120179

13
Gas phase Energy: -1016.72022467762 hartrees
Solvation Energy: -0.00614492515 hartrees
Zero Point Energy: 305.764 kcal/mol
Free Energy: -30.671 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.3183014850	0.3244792272	0.0235212892
C2	0.1544409878	-0.1073167880	3.6338970441
C3	2.3052210435	-0.0364706301	2.4538113987
C4	1.8431563812	-1.2084628136	1.5651279905
N5	0.3655510631	-1.3567942307	1.4366852676
C6	-0.3064876247	-1.3083205704	2.7743384780
C7	-1.8257582979	-1.4254173096	2.6008124178
C8	-2.1932061588	-2.7511235717	1.9174415235
C9	-1.4185187402	-2.9067434877	0.6015807850
C10	0.0790680057	-2.6708738709	0.8004626833
C11	1.6709128122	-0.2078352784	3.8419614835
C12	-0.1746979216	1.3040598787	3.1093312049
N13	0.5464528444	1.6439778067	1.8672836366
C14	2.0121502511	1.3766608099	1.8944912586
C15	2.8262415254	2.4680550529	2.6325762031
C16	0.9936043376	4.1271805545	2.1571726664
C17	2.5057988451	3.8729568805	2.0999585221
C18	0.2501715986	3.0196528332	1.3955350334
H19	-0.3623694496	-0.2123942392	4.5967588942
H20	3.3968982600	-0.1273544426	2.5248318087
H21	2.2485956385	-1.1145725331	0.5532176558
H22	2.2607556753	-2.1330706254	2.0054230256
H23	0.0242113790	-2.2047541331	3.3366452794
H24	-2.3019015028	-1.3569216404	3.5871106181
H25	-2.1838365904	-0.5837419274	1.9951900305
H26	-1.9494053725	-3.5847933907	2.5913923563
H27	-3.2722638420	-2.8022343472	1.7330162289
H28	-1.5643031446	-3.9092110117	0.1807004368
H29	-1.7872714685	-2.1819992824	-0.1306986731
H30	0.6018304047	-2.6934327956	-0.1600116925
H31	0.5027056338	-3.4753010753	1.4315334806
H32	2.0207564729	0.5554129869	4.5447568064
H33	1.9413869830	-1.1821695799	4.2678422645
H34	0.0485055946	2.0111898696	3.9282675014
H35	-1.2438612922	1.3999563554	2.8937501888

H36	2.3252260307	1.3988297389	0.8408369514
H37	3.8948447148	2.2472461085	2.5142555460
H38	2.6202007149	2.4405426009	3.7099448820
H39	0.7426700765	5.0961570774	1.7091168292
H40	0.6616978476	4.1710197373	3.2034727158
H41	2.8452641725	3.9555220037	1.0575283483
H42	3.0552276552	4.6308687457	2.6705728402
H43	-0.8343366840	3.1580279594	1.4415104657
H44	0.5224551993	3.0629949935	0.3348882092
O45	-0.8963942934	1.4826077774	-1.5913875502
C46	-1.0422588799	0.2480684281	-1.9819268608
C47	-2.4631149461	-0.2782277223	-2.1591682693
C48	-0.0219005166	-0.3295284283	-2.9587961369
H49	-3.1181666245	0.1220042145	-1.3820820085
H50	-2.8574044927	0.0413892748	-3.1364697965
H51	-2.5041718134	-1.3726403835	-2.1391406214
H52	0.9680122760	0.0901348144	-2.7651554470
H53	0.0319740224	-1.4219653125	-2.8918426156
H54	-0.3047961076	-0.0803279948	-3.9939269360

14_{trip}
Gas phase Energy: -1167.03756580482 hartrees
Solvation Energy: -0.00591068334 hartrees
Zero Point Energy: 308.354 kcal/mol
Free Energy: -34.813 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.5142570733	0.4266884448	0.0372289759
C2	0.1129265813	-0.0541855105	3.6236477185
C3	2.2050133396	0.0001047058	2.3418486098
C4	1.6905370538	-1.1601469732	1.4674994786
N5	0.2075765930	-1.2802969726	1.3987838298
C6	-0.4071959388	-1.2321160745	2.7654084569
C7	-1.9346866720	-1.3148806255	2.6547779071
C8	-2.3592114107	-2.6264197019	1.9775712985
C9	-1.6428750040	-2.7872681405	0.6298305272
C10	-0.1333759876	-2.5839421897	0.7677311628
C11	1.6358681337	-0.1780991140	3.7570047116
C12	-0.2194506635	1.3705712846	3.1410420355
N13	0.4384832773	1.7124606719	1.8669087502
C14	1.8989602720	1.4208613506	1.8085672387
C15	2.7710008629	2.4948213214	2.5047800791
C16	0.9424815900	4.1863019667	2.1406518257
C17	2.4444707063	3.9070977047	1.9960835308
C18	0.1380526831	3.0946917303	1.4188244627

H19	-0.3589812505	-0.1711718689	4.6080543709
H20	3.2979033445	-0.1008491631	2.3605713810
H21	2.0572423976	-1.0687464514	0.4409731103
H22	2.1096906203	-2.0935247361	1.8875742673
H23	-0.0724079663	-2.1429860109	3.3012575384
H24	-2.3677987371	-1.2443319589	3.6605017890
H25	-2.2990143985	-0.4608275024	2.0708218845
H26	-2.1062717526	-3.4708517519	2.6345968441
H27	-3.4459310851	-2.6526704586	1.8374965798
H28	-1.8268226794	-3.7831475225	0.2086977887
H29	-2.0268338728	-2.0499825493	-0.0818993150
H30	0.3471630420	-2.6129859597	-0.2138814779
H31	0.2985006421	-3.4013610123	1.3766070834
H32	2.0293129000	0.5731038779	4.4498632385
H33	1.9133687518	-1.1605167519	4.1592022279
H34	0.0611709072	2.0610139423	3.9569248571
H35	-1.2970593117	1.4885831006	2.9864525336
H36	2.1510901005	1.4447012657	0.7387623617
H37	3.8276304387	2.2568438242	2.3257166214
H38	2.6248017940	2.4647807979	3.5921478173
H39	0.6827389364	5.1614079911	1.7107849738
H40	0.6717689420	4.2306927745	3.2045552152
H41	2.7250194622	3.9876915444	0.9359060071
H42	3.0386378845	4.6534867539	2.5363993820
H43	-0.9395780973	3.2506807571	1.5281411288
H44	0.3481876761	3.1391489983	0.3441241099
O45	-1.1976696091	1.6464157216	-1.4855719875
C46	-1.2367062140	0.4396671433	-1.9741011756
C47	-2.5999248808	-0.2057130924	-2.1977172440
C48	-0.1663340457	0.0463652461	-2.9882623628
H49	-3.2899838742	0.0659261158	-1.3957957247
H50	-3.0264755547	0.1450979847	-3.1504271186
H51	-2.5282407562	-1.2970171527	-2.2579865338
H52	0.7728440180	0.5546269513	-2.7596208219
H53	0.0064556440	-1.0331507676	-3.0071445922
H54	-0.4806168717	0.3440119317	-4.0016850006
O55	-0.5991057317	-3.7629102204	-2.6099079745
O56	0.0365017680	-3.5563699488	-3.6233967934

15_{trip}
Gas phase Energy: -1167.05254091834 hartrees
Solvation Energy: -0.00730906375 hartrees
Zero Point Energy: 309.645 kcal/mol
Free Energy: -33.946 kcal/mol
final geometry:
angstroms

atom	x	y	z
Pd1	-0.7132900524	-0.2177960696	0.3881724256
C2	0.5344304176	-0.1212517838	3.6480165509
C3	2.3316982400	0.1098968234	1.9872430032
C4	1.9181703088	-1.2386762940	1.3701699337
N5	0.4918786843	-1.5994549978	1.6072387933
C6	0.1228197975	-1.4913114688	3.0555686605
C7	-1.3551479702	-1.8541452933	3.2594275712
C8	-1.6600850248	-3.2691768118	2.7447182204
C9	-1.2055734094	-3.4208598574	1.2865196817
C10	0.2523900450	-2.9894853585	1.1195330080
C11	2.0525488977	0.0471630902	3.4969833581
C12	-0.1549354597	1.1281669461	3.0615300495
N13	0.1824699028	1.3725237679	1.6329307531
C14	1.6660231626	1.3559786254	1.3506824749
C15	2.3831016469	2.6595143857	1.7746689695
C16	0.2260397639	3.9250937129	1.5892617277
C17	1.7058434250	3.9059129988	1.1882716493
C18	-0.4499424451	2.6314535385	1.1189819278
H19	0.2638043964	-0.1556714043	4.7112129120
H20	3.4096093491	0.2078698897	1.8069186250
H21	2.0773639034	-1.2390034786	0.2878817640
H22	2.5646509291	-2.0224473648	1.8032560163
H23	0.7242766765	-2.2439095081	3.6008855192
H24	-1.5869499733	-1.7752475588	4.3290822712
H25	-1.9850219886	-1.1294848914	2.7296780852
H26	-1.1379633185	-4.0043797128	3.3740139031
H27	-2.7311081795	-3.4813808918	2.8351657455
H28	-1.2967793845	-4.4635945608	0.9595616179
H29	-1.8339286842	-2.8144122471	0.6238525227
H30	0.5429188672	-3.0183890498	0.0656056850
H31	0.9179162055	-3.6749422003	1.6742334271
H32	2.3983862845	0.9492185521	4.0114996422
H33	2.5834536714	-0.8002571494	3.9480153043
H34	0.1394667189	1.9853468706	3.6864852841
H35	-1.2438229553	1.0467133576	3.1231851284
H36	1.7422755389	1.2860544440	0.2596168110
H37	3.4236713878	2.5931482361	1.4336119873
H38	2.4196563473	2.7515018133	2.8676771056
H39	-0.2955824182	4.7703529505	1.1247442585
H40	0.1263358100	4.0566621082	2.6754621799
H41	1.7801414065	3.8807031377	0.0938039923
H42	2.2186902881	4.8120730600	1.5312518882
H43	-1.5071012831	2.5969494993	1.3983737275
H44	-0.3939480438	2.5819762105	0.0289655396
O45	1.0559852799	1.9732648423	-1.9610252331

C46	0.2933612966	1.5171655503	-2.8053694539
C47	-0.8294674113	2.3500907675	-3.3887768518
C48	0.4108000247	0.0926689479	-3.2955178038
H49	-0.8043172586	3.3597772709	-2.9743332583
H50	-0.7527563863	2.3964124587	-4.4814750296
H51	-1.7783651287	1.8673275379	-3.1344531175
H52	-0.3181834898	-0.5115797755	-2.7322451062
H53	0.1729453588	0.0055684565	-4.3607989650
H54	1.4174169804	-0.2862852382	-3.1032128423
O55	-1.7699487028	-0.9988167329	-1.1380462403
O56	-1.9611626927	0.3817744086	-1.0684761675

16_{trip}
Gas phase Energy: -1167.05396100073 hartrees
Solvation Energy: -0.00859357794 hartrees
Zero Point Energy: 308.435 kcal/mol
Free Energy: -35.829 kcal/mol
final geometry:

	angstroms		
atom	x	y	z
Pd1	-0.4355507075	-0.4079781964	0.0403669130
C2	0.1209177723	0.3261059510	3.5222353713
C3	2.2572279569	0.3328692856	2.3103920484
C4	1.9755235311	-1.1032949134	1.8303490610
N5	0.5364320603	-1.4804796497	1.8074658985
C6	-0.1565481360	-1.1328165114	3.0857578380
C7	-1.6440226239	-1.4999402015	2.9916388061
C8	-1.8283749437	-2.9967253136	2.6967169015
C9	-1.0254388597	-3.4065240103	1.4540146088
C10	0.4286146964	-2.9437372987	1.5607689439
C11	1.6338354149	0.5013838133	3.7036722254
C12	-0.3923800267	1.4529940751	2.6016830678
N13	0.2862410320	1.4962785036	1.2870296631
C14	1.7778444421	1.4558307017	1.3588210592
C15	2.4138343256	2.8212216109	1.7197725674
C16	0.3806707347	4.0007479448	0.8166106539
C17	1.9135242374	3.9476011490	0.8031789934
C18	-0.1866311376	2.6256898022	0.4411254024
H19	-0.3885247176	0.4543288756	4.4861889890
H20	3.3495114763	0.4204701860	2.3741878811
H21	2.3685348966	-1.2613741463	0.8209440671
H22	2.5187137945	-1.7887155788	2.5069660613
H23	0.2849107811	-1.7639718977	3.8830950774
H24	-2.1334899653	-1.2321210012	3.9365100311
H25	-2.1110562244	-0.9076287740	2.1944380077
H26	-1.4864596211	-3.5807345753	3.5631551772

H27	-2.8901378827	-3.2301895095	2.5597937061
H28	-1.0387115483	-4.4955713344	1.3251904774
H29	-1.4712952491	-2.9667525155	0.5536381793
H30	0.9700660202	-3.1632551623	0.6356445385
H31	0.9355906639	-3.4847908100	2.3816167442
H32	1.8653832945	1.4804379434	4.1353168937
H33	2.0326544547	-0.2531745073	4.3933786322
H34	-0.2686617919	2.3996799654	3.1549899000
H35	-1.4630968015	1.3409976713	2.4045951521
H36	2.1067942632	1.2069701355	0.3401792813
H37	3.5048432927	2.7226984650	1.6493840080
H38	2.1929887436	3.0849894178	2.7617197310
H39	0.0103552875	4.7272651697	0.0857296174
H40	0.0223659774	4.3205443490	1.8049473277
H41	2.2536420245	3.7669680529	-0.2258196195
H42	2.3441409332	4.9068670622	1.1134264379
H43	-1.2805013553	2.6207891047	0.4693599151
H44	0.1033191903	2.4048551612	-0.5896331202
O45	-1.4694518104	-1.2754511409	-1.8866634683
O46	-1.3961361631	0.0346921868	-1.8161562849
O47	-0.3023813587	3.8343997030	-2.6782099714
C48	-0.8938372966	3.0431972567	-3.3954152245
C49	-2.4034143288	2.9083560784	-3.3633652582
C50	-0.1513514960	2.1004283419	-4.3224078492
H51	-2.6515445277	1.9142837792	-2.9715909208
H52	-2.8345758912	3.6790459746	-2.7219528164
H53	-2.8286241547	2.9788526532	-4.3709760933
H54	0.9110673023	2.3501390476	-4.3380051141
H55	-0.2867640228	1.0771432908	-3.9513836895
H56	-0.5605834955	2.1354738402	-5.3382778780

$Pd(Cl)(O_2)^-$ trip
Gas phase Energy: -1434.17876148788 hartrees
Solvation Energy: -0.04658614061 hartrees
Zero Point Energy: 254.048 kcal/mol
Free Energy: -32.772 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-2.1577589331	1.1950863160	1.2769206144
C2	1.7636712044	-0.6996880788	2.8890532480
C3	2.0064130598	-0.4129619852	0.4620754455
C4	0.7720237590	-1.3097748239	0.2492920114
N5	-0.1311510167	-1.3673714192	1.3970407732
C6	0.5353212359	-1.6203136136	2.6793486765
C7	-0.4837280274	-1.5402948325	3.8265671952

C8	-1.6319711327	-2.5361323638	3.6159799827
C9	-2.2734767713	-2.2977093410	2.2441854228
C10	-1.2204195927	-2.3098198743	1.1339653723
C11	2.7393074601	-0.8956494355	1.7221959488
C12	1.4854545726	0.8104163575	3.0382407020
N13	1.0010374508	1.4310624706	1.8107037588
C14	1.6900346838	1.0988487034	0.5566166425
C15	2.9576636494	1.9646885953	0.3166587476
C16	1.9526365307	3.7599971952	1.7842795968
C17	2.6461368481	3.4652253596	0.4452705413
C18	0.7104260454	2.8589989702	1.9314979883
H19	2.2337293960	-1.0261671897	3.8276006499
H20	2.6464963996	-0.5499412587	-0.4209301691
H21	0.1886860176	-0.9609858767	-0.6090757507
H22	1.1508729982	-2.3273110710	-0.0038155743
H23	0.9501807551	-2.6591452388	2.6823042882
H24	0.0329907054	-1.7408895595	4.7758803241
H25	-0.9029177459	-0.5294835821	3.8758248798
H26	-1.2451030115	-3.5665616826	3.6709668871
H27	-2.3773289555	-2.4297728227	4.4132538166
H28	-3.0337901108	-3.0601891389	2.0273417436
H29	-2.7740353332	-1.3211379127	2.2440113232
H30	-1.6822273331	-2.0178904014	0.1852680655
H31	-0.8201407227	-3.3436404140	1.0144519952
H32	3.6685887172	-0.3375838266	1.8934994061
H33	3.0130710884	-1.9545972436	1.6181484162
H34	2.4276717548	1.2648169583	3.4162253323
H35	0.7276085474	0.9868270048	3.8095380989
H36	0.9767780398	1.3393640560	-0.2465165046
H37	3.3644113729	1.7445194686	-0.6803870891
H38	3.7400804724	1.6987345395	1.0408290176
H39	1.6566865377	4.8158528678	1.8456996674
H40	2.6530912685	3.5790750905	2.6122972295
H41	1.9763314080	3.7648066859	-0.3745305076
H42	3.5632323987	4.0597032149	0.3344279847
H43	0.1990054966	3.0269294051	2.8843832711
H44	-0.0113056193	3.1233466403	1.1447056269
Cl45	-2.8768116783	1.6132852553	3.5866166888
O46	-1.6671408249	1.0871208369	-0.6763950473
O47	-2.0974818767	-0.0119896442	-1.2330289685

Pd(tol)
Gas phase Energy: -1095.12131467596 hartrees
Solvation Energy: -0.00243613355 hartrees
Zero Point Energy: 332.300 kcal/mol
Free Energy: -32.732 kcal/mol

final geometry:

	angstroms		
atom	x	y	z
Pd1	-0.7614102957	0.2448645138	-0.1140171120
C2	0.2444604369	-0.1425894763	3.5558138332
C3	2.1908048844	0.3756282917	2.1567950310
C4	1.8744714044	-0.8532552384	1.2833428745
N5	0.4628732785	-1.3086462528	1.3286616173
C6	-0.0532069537	-1.4081407107	2.7215642419
C7	-1.5303977861	-1.8211143089	2.6991187384
C8	-1.6968674689	-3.1901897164	2.0238760767
C9	-1.0562120422	-3.1707926994	0.6297987008
C10	0.3764356873	-2.6361219680	0.6745313538
C11	1.7632025666	0.0638712233	3.5985761690
C12	-0.4224628009	1.1705198034	3.1016551072
N13	0.0781629248	1.6774589026	1.8074109941
C14	1.5638351694	1.7081634114	1.6816882885
C15	2.2279737734	2.9188242293	2.3876420891
C16	0.0679845986	4.1905679827	2.2143174548
C17	1.5830755641	4.2516532793	1.9823199689
C18	-0.5202723815	2.9874402179	1.4592095415
H19	-0.1333224983	-0.3502564160	4.5657830135
H20	3.2797390781	0.5073314330	2.1081927418
H21	2.1183752258	-0.6552693762	0.2342979508
H22	2.5370393490	-1.6713052662	1.6273405850
H23	0.5001313085	-2.2241235725	3.2331700767
H24	-1.9106927828	-1.8494443372	3.7282579711
H25	-2.1045410666	-1.0648971354	2.1482844660
H26	-1.2152909482	-3.9600231506	2.6438075993
H27	-2.7569359355	-3.4608110120	1.9542448107
H28	-1.0467547675	-4.1756422837	0.1894899899
H29	-1.6431106673	-2.5248964959	-0.0303938820
H30	0.7733617564	-2.5318439516	-0.3398252497
H31	1.0245009626	-3.3544234954	1.2150366897
H32	2.0315111881	0.8711778941	4.2880275961
H33	2.2667741724	-0.8423688764	3.9583151287
H34	-0.2731935135	1.9003313038	3.9177150303
H35	-1.5045057440	1.0374044356	2.9959466146
H36	1.7577037518	1.8145057728	0.6048267413
H37	3.2978595468	2.9195259293	2.1421325884
H38	2.1605664641	2.8127028942	3.4775370064
H39	-0.4205444818	5.1069636075	1.8606330230
H40	-0.1431551237	4.1195225740	3.2899377459
H41	1.7778931361	4.4462839847	0.9178539575
H42	2.0359763205	5.0792817596	2.5412372170
H43	-1.6015383621	2.9088793044	1.6135413454

H44	-0.3626190229	3.1352860064	0.3852097200
C45	-1.5810941777	-0.1448304356	-2.1172356197
C46	-1.6443637536	1.2629860610	-1.7992067082
C47	-2.8373713620	-0.9983873813	-2.0776211081
C48	-0.6765623742	2.1560193961	-2.3625924733
C49	0.3460228726	1.6888839189	-3.1630898196
C50	0.4463840794	0.3034051872	-3.4426651870
C51	-0.4862370967	-0.5806264756	-2.9375430543
H52	-3.4082660019	-0.8861447199	-3.0107577973
H53	-2.5982178610	-2.0620387644	-1.9750434732
H54	-3.4942222459	-0.7173559862	-1.2502333545
H55	-2.5846532991	1.6856696175	-1.4448224229
H56	-0.7824801829	3.2241969653	-2.1839838218
H57	1.0672517312	2.3815395273	-3.5896513383
H58	1.2527413754	-0.0626092965	-4.0737290716
H59	-0.4343462163	-1.6339290006	-3.2097117874

TRS2-3
Gas phase Energy: -1458.85113824769 hartrees
Solvation Energy: -0.01403913521 hartrees
Zero Point Energy: 336.330 kcal/mol
Free Energy: -34.930 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-1.0480201060	-1.0491305974	-0.8281607684
C2	-1.2868205880	2.7566862820	-1.3114473117
C3	-2.6955471087	2.0279363413	0.5599129743
C4	-3.3750180917	0.9915675041	-0.3564192768
N5	-2.5687396084	0.5482431444	-1.5266842679
C6	-1.9554207452	1.7169023490	-2.2426539593
C7	-1.0627446402	1.1993012167	-3.3768725620
C8	-1.8944262183	0.4046032646	-4.3963449824
C9	-2.7023354781	-0.6956282215	-3.6919824915
C10	-3.4668024882	-0.1463973754	-2.4847204586
C11	-2.3227129359	3.2486904535	-0.2933632649
C12	-0.0266502536	2.3248596538	-0.5410992855
N13	-0.3053329963	1.3109939070	0.4683168649
C14	-1.4651749643	1.5194476769	1.3490964454
C15	-1.1497438099	2.4268644427	2.5674075816
C16	1.2784556580	1.7555414246	2.3735774914
C17	0.0878984858	1.9249125782	3.3294663130
C18	0.8772085382	0.8447632772	1.1999796044
H19	-0.9884479922	3.5847712659	-1.9685586311
H20	-3.4558134517	2.3078908810	1.3017049429
H21	-3.6461558625	0.0939518115	0.2069001743

H22	-4.3131819631	1.4560432605	-0.7189043961
H23	-2.7915324814	2.2722751779	-2.7156149461
H24	-0.5702009194	2.0496041892	-3.8660320023
H25	-0.2874275779	0.5533550836	-2.9455814253
H26	-2.5786983369	1.0891251254	-4.9183283127
H27	-1.2451555561	-0.0351935792	-5.1626366823
H28	-3.4154051512	-1.1597583757	-4.3869340888
H29	-2.0164861114	-1.4699034235	-3.3232744781
H30	-3.9652951634	-0.9560870844	-1.9419363987
H31	-4.2534880503	0.5554474724	-2.8264630141
H32	-1.9082647160	4.0571482868	0.3192005742
H33	-3.2117874062	3.6500223698	-0.7974213982
H34	0.4218235655	3.2519246170	-0.1268206018
H35	0.7179661550	1.9039179881	-1.2272438646
H36	-1.7113843994	0.5212736264	1.7463427984
H37	-2.0223878164	2.4562540706	3.2345110865
H38	-0.9729564628	3.4593192611	2.2364349559
H39	2.1383501073	1.3206999913	2.8988904447
H40	1.5995007385	2.7398526208	2.0036714429
H41	-0.1411810739	0.9520913921	3.7895041741
H42	0.3344943199	2.6095847518	4.1506912150
H43	1.6982132761	0.7305634269	0.4847365271
H44	0.6617312302	-0.1641084626	1.5740773454
H45	-1.2518025763	-3.4306818745	-0.6153739430
Cl46	0.6041644666	-2.6436940773	-0.0285708658
N47	-1.9250326499	-4.2721713142	-0.5263306978
C48	-2.8039020052	-4.2664948467	-1.7248783212
C49	-1.0948045844	-5.5050821482	-0.4364781191
C50	-2.6876056141	-4.0116204787	0.7268235347
H51	-3.2823460370	-3.2898087036	-1.7856125223
H52	-2.1860748120	-4.4116038489	-2.6096899229
H53	-3.5419600968	-5.0660076775	-1.6411715924
H54	-0.5051504566	-5.5948428550	-1.3511123972
H55	-0.4148209564	-5.3967941469	0.4089429106
H56	-1.7461138395	-6.3763895171	-0.3138063662
H57	-3.1338470987	-3.0189810375	0.6398500889
H58	-3.4478008663	-4.7855835583	0.8617828965
H59	-1.9832082878	-4.0063704203	1.5588502216

TRS7-8
Gas phase Energy: -1434.73743676416 hartrees
Solvation Energy: -0.01818562421 hartrees
Zero Point Energy: 264.952 kcal/mol
Free Energy: -28.784 kcal/mol
final geometry:
angstroms

atom	x	y	z
Pd1	-0.5474179360	-0.2758658731	0.0894202520
C2	-0.0628601116	-0.1044908333	3.5086180390
C3	2.0499406902	-0.0775466650	2.2510005362
C4	1.6663340747	-1.4185421890	1.5970431523
N5	0.1896551269	-1.6746447702	1.5527011848
C6	-0.4474065249	-1.4717699275	2.8972189820
C7	-1.9542055087	-1.7473644488	2.8293259125
C8	-2.2311122925	-3.1815472506	2.3557233664
C9	-1.5315291596	-3.4430932123	1.0157903933
C10	-0.0476730707	-3.0754486669	1.0743706304
C11	1.4627923857	-0.0465714830	3.6707205696
C12	-0.5277520597	1.1454989501	2.7356755240
N13	0.1238576723	1.2925537378	1.4035707344
C14	1.6319710056	1.1805237291	1.4513909366
C15	2.3151911845	2.4599256583	1.9816740105
C16	0.3378956375	3.8312426873	1.2625938279
C17	1.8654313293	3.7099475672	1.2128496245
C18	-0.3047151112	2.5549452872	0.7084409170
H19	-0.5490463011	-0.0631902214	4.4914149736
H20	3.1458076445	-0.0681852484	2.2933038966
H21	2.0370455582	-1.4777735961	0.5701875575
H22	2.1377844474	-2.2287972717	2.1769966064
H23	-0.0060457530	-2.2328134568	3.5662109466
H24	-2.3808681815	-1.5793314193	3.8257627201
H25	-2.4282238779	-1.0338587435	2.1437468462
H26	-1.8674079396	-3.8890994142	3.1144313281
H27	-3.3093869463	-3.3486587098	2.2611387966
H28	-1.6049179338	-4.5015766933	0.7403955954
H29	-2.0100445085	-2.8688042106	0.2165996042
H30	0.4108935391	-3.1613220128	0.0860773213
H31	0.4854403868	-3.7547890089	1.7601232880
H32	1.7641037275	0.8542904261	4.2135749998
H33	1.8215367481	-0.9034351297	4.2537735678
H34	-0.3138902776	2.0221274369	3.3629297399
H35	-1.6081352917	1.1296198511	2.5646357945
H36	1.9270576664	1.0561981556	0.4025340544
H37	3.3984044117	2.3198860583	1.8837065733
H38	2.1151103782	2.6033749908	3.0511666799
H39	-0.0078703710	4.6725272025	0.6513218902
H40	0.0040806150	4.0331981110	2.2896862088
H41	2.1879002206	3.6329641757	0.1670845251
H42	2.3410039607	4.6028007272	1.6340203513
H43	-1.3976144449	2.5949700676	0.7623906795
H44	-0.0159436193	2.4341310776	-0.3412722353
O45	-1.2482162012	-1.3965446090	-1.3708385824

O46	-1.5998839840	-0.1447503748	-1.9269832982
H47	-0.7359757313	0.1654064498	-2.3562563431
Cl48	1.1418731910	0.9298348885	-2.1806341313

TRS14-15
Gas phase Energy: -1167.03278815351 hartrees
Solvation Energy: -0.00480795676 hartrees
Zero Point Energy: 308.375 kcal/mol
Free Energy: -33.751 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.4991741461	0.1560398936	0.0366385691
C2	0.1086622710	0.0143955062	3.6645981852
C3	2.2198795345	-0.0015895036	2.4136239354
C4	1.7420511269	-1.2374383341	1.6264890801
N5	0.2627369619	-1.3973414547	1.5455655071
C6	-0.3848481301	-1.2299754046	2.8897171390
C7	-1.9088077592	-1.3340402925	2.7472161494
C8	-2.3098326515	-2.7044341065	2.1796310150
C9	-1.5451432435	-2.9956176391	0.8806369725
C10	-0.0424598253	-2.7681806271	1.0518949072
C11	1.6305189877	-0.0793240846	3.8298072192
C12	-0.2324697518	1.3950540635	3.0762228872
N13	0.4411471198	1.6541197977	1.7926763709
C14	1.9027485604	1.3700938106	1.7687922324
C15	2.7599593129	2.5014134450	2.3900857937
C16	0.9182499376	4.1429682279	1.8933497277
C17	2.4239562713	3.8702467544	1.7799464883
C18	0.1303555564	2.9951501461	1.2450346329
H19	-0.3776567899	-0.0368879773	4.6476181712
H20	3.3138524295	-0.0818884545	2.4572991529
H21	2.1237756351	-1.2229398761	0.6014083026
H22	2.1727920021	-2.1242873933	2.1269113422
H23	-0.0587270691	-2.0907447233	3.5063379325
H24	-2.3694987225	-1.1760091933	3.7307099959
H25	-2.2616385973	-0.5372295881	2.0800198988
H26	-2.0823825782	-3.4816388852	2.9232400602
H27	-3.3910927791	-2.7454316427	2.0048066201
H28	-1.7093905800	-4.0300294483	0.5561118288
H29	-1.9040804231	-2.3406177789	0.0789769390
H30	0.4739048514	-2.9072298384	0.1008978160
H31	0.3684875079	-3.5029082298	1.7694440098
H32	2.0032450511	0.7275689627	4.4695177036
H33	1.9139670147	-1.0244757482	4.3096863454
H34	0.0254955987	2.1459450280	3.8451709921

H35	-1.3091681058	1.4875723536	2.8979911390
H36	2.1668822627	1.3151581159	0.7026600072
H37	3.8199994366	2.2619767611	2.2358172740
H38	2.6059018449	2.5477517451	3.4756516735
H39	0.6524434097	5.0829243206	1.3944505436
H40	0.6393861117	4.2595450436	2.9496073619
H41	2.7127066258	3.8786795910	0.7190013039
H42	3.0063095907	4.6590932822	2.2704648378
H43	-0.9495056864	3.1471738949	1.3360383664
H44	0.3425789277	2.9664714842	0.1708632639
O45	-1.2386427338	1.6140541567	-1.2638834725
C46	-1.2714738685	0.7153451535	-2.1656152764
C47	-2.5796069181	0.0283065075	-2.5087823436
C48	-0.1791878502	0.6737836648	-3.2129453290
H49	-3.2526049976	0.0398206682	-1.6494709994
H50	-3.0635785226	0.5683034410	-3.3377410628
H51	-2.4191583821	-0.9998756699	-2.8413443293
H52	0.7234783369	1.1569606063	-2.8338592853
H53	0.0462046949	-0.3463498056	-3.5331495487
H54	-0.5198610797	1.2219151744	-4.1050466997
O55	-0.3316649928	-2.4587427842	-2.0061680652
O56	-0.1333106968	-2.5658555910	-3.2242443881

TRS15-16
Gas phase Energy: -1167.04867474454 hartrees
Solvation Energy: -0.00877085882 hartrees
Zero Point Energy: 308.372 kcal/mol
Free Energy: -35.138 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.1638547897	-0.0022318294	0.0444644103
C2	-0.0212010556	0.1692019555	3.6924706980
C3	2.2212181393	0.0463920208	2.7070766011
C4	1.8455838333	-1.2961940278	2.0495471193
N5	0.3924889591	-1.4989773946	1.8532188275
C6	-0.4005820619	-1.1973421707	3.0734000016
C7	-1.8983311876	-1.3634802716	2.7847817833
C8	-2.2086905223	-2.7952507820	2.3263360430
C9	-1.3333781811	-3.1668657100	1.1228895672
C10	0.1471548158	-2.8871281230	1.3938251077
C11	1.4712140616	0.1479193079	4.0437404836
C12	-0.3142538680	1.4337627837	2.8581056187
N13	0.5108002558	1.5582056107	1.6283622139
C14	1.9771738016	1.3147202107	1.8493113241
C15	2.7303049362	2.5315058982	2.4454023742

C16	0.9543292967	4.0732802209	1.5795984806
C17	2.4643606206	3.8267562407	1.6674720585
C18	0.2683978709	2.8595202355	0.9394739571
H19	-0.6195646065	0.2626208302	4.6082333658
H20	3.3032956578	0.0015655504	2.8859949075
H21	2.3254771063	-1.3976984426	1.0703747648
H22	2.2490367592	-2.0991912005	2.6965611736
H23	-0.1362787493	-1.9479728946	3.8478048579
H24	-2.4633933986	-1.1155674150	3.6924219220
H25	-2.1948501798	-0.6539732219	2.0015918138
H26	-2.0158641528	-3.4895367861	3.1572789137
H27	-3.2705820301	-2.8956260069	2.0736350781
H28	-1.4442593371	-4.2297622274	0.8761983863
H29	-1.6393671922	-2.5999448700	0.2386698345
H30	0.7225842619	-3.0371293310	0.4757023545
H31	0.5307130380	-3.5927874040	2.1562333620
H32	1.7566417521	1.0428691872	4.6062174845
H33	1.7071896733	-0.7156076837	4.6778709897
H34	-0.1619174713	2.2977978709	3.5263637299
H35	-1.3609169612	1.4603430114	2.5406268533
H36	2.3889718852	1.1392442632	0.8464663405
H37	3.8023539054	2.2974717049	2.4487336769
H38	2.4444005546	2.6860675884	3.4929667793
H39	0.7335550606	4.9581617767	0.9705198455
H40	0.5489051986	4.2747552100	2.5803408557
H41	2.8770836345	3.7409937748	0.6521218484
H42	2.9772805370	4.6691441892	2.1462282187
H43	-0.8135986260	2.9927457658	0.8695479238
H44	0.6242687700	2.7497895790	-0.0895305544
O45	-1.4657256610	1.8131695016	-1.4143437891
C46	-1.8974268313	1.4595177565	-2.5090612961
C47	-3.0858639258	0.5276241830	-2.6331269845
C48	-1.2673903859	1.9462505887	-3.8018613013
H49	-3.4592817425	0.2632161589	-1.6384103881
H50	-3.8884218253	0.9974904365	-3.2209834023
H51	-2.7703360786	-0.3806580891	-3.1576245037
H52	-0.5205522190	2.7146869321	-3.5916679601
H53	-0.7786829409	1.0959263595	-4.2860491319
H54	-2.0245086491	2.3359549762	-4.4935863124
O55	-0.4175088025	-1.4451809999	-1.4265395484
O56	-0.3484401550	-0.9186789738	-2.6232025658

MECP4
Gas phase Energy: -1609.20132792015 hartrees
Solvation Energy: -0.01426722307 hartrees
Zero Point Energy: 341.483 kcal/mol

Free Energy: -35.330 kcal/mol

final geometry:

	angstroms		
atom	x	y	z
Pd1	-1.3639345000	0.7445760000	1.4417436000
C2	1.6204488000	-0.6752606000	3.0024584000
C3	1.9512198000	-0.3146785000	0.6043922000
C4	0.7375914000	-1.2186448000	0.3168513000
N5	-0.2448376000	-1.3306612000	1.4278936000
C6	0.4333324000	-1.6216850000	2.7234058000
C7	-0.6016438000	-1.7088713000	3.8506697000
C8	-1.5452653000	-2.8935826000	3.5950317000
C9	-2.2025238000	-2.7509895000	2.2144227000
C10	-1.1910007000	-2.4403908000	1.1053711000
C11	2.6463965000	-0.8288022000	1.8752889000
C12	1.3169336000	0.8223093000	3.1820345000
N13	0.8499336000	1.5075033000	1.9512362000
C14	1.6586230000	1.1998582000	0.7256902000
C15	2.9783995000	2.0052299000	0.6057452000
C16	2.0770162000	3.7323441000	2.1692255000
C17	2.7855182000	3.5079979000	0.8297547000
C18	0.7422691000	2.9772311000	2.1733058000
H19	2.0486882000	-1.0140463000	3.9548118000
H20	2.6169228000	-0.4285737000	-0.2605384000
H21	0.1953585000	-0.8755156000	-0.5711842000
H22	1.1372395000	-2.2251778000	0.0921970000
H23	0.8924116000	-2.6279118000	2.6342753000
H24	-0.0708870000	-1.8268556000	4.8045848000
H25	-1.1740353000	-0.7729881000	3.8983198000
H26	-0.9642484000	-3.8268665000	3.6604915000
H27	-2.3185290000	-2.9458613000	4.3708490000
H28	-2.7135589000	-3.6814639000	1.9337147000
H29	-2.9607957000	-1.9596792000	2.2476387000
H30	-1.7259089000	-2.1551589000	0.1956366000
H31	-0.5869200000	-3.3416813000	0.8872500000
H32	3.5598398000	-0.2688154000	2.0981805000
H33	2.9425342000	-1.8778608000	1.7549898000
H34	2.2393357000	1.2860672000	3.5678796000
H35	0.5441436000	0.9730015000	3.9420566000
H36	1.0185613000	1.4971790000	-0.1160833000
H37	3.3911031000	1.8133945000	-0.3927888000
H38	3.7237100000	1.6359678000	1.3208410000
H39	1.8741797000	4.7966062000	2.3333051000
H40	2.7271710000	3.4075771000	2.9934361000
H41	2.1805781000	3.9354399000	0.0175135000
H42	3.7531148000	4.0208804000	0.8017486000

H43	0.1957029000	3.1242062000	3.1089965000
H44	0.1013813000	3.3776024000	1.3847761000
H45	-4.3115624000	2.6169223000	1.2359351000
Cl46	-2.4213072000	3.0977522000	1.1281684000
N47	-5.3758938000	2.5736147000	1.3127765000
C48	-5.8357218000	1.5677969000	0.3058044000
C49	-5.6778279000	2.1318739000	2.7078792000
C50	-5.8627683000	3.9493437000	1.0302299000
H51	-5.4206852000	1.8460439000	-0.6642150000
H52	-5.4320285000	0.6032471000	0.6234790000
H53	-6.9303100000	1.5630093000	0.2716540000
H54	-5.2721811000	2.8689730000	3.4025012000
H55	-6.7609914000	2.0500537000	2.8285604000
H56	-5.1693603000	1.1696418000	2.8248738000
H57	-5.4230115000	4.6412461000	1.7497179000
H58	-5.5468086000	4.2401230000	0.0283209000
H59	-6.9527465000	3.9702287000	1.1011423000
O60	-3.1115154000	-0.0500439000	0.8569847000
O61	-3.9542412000	-0.2309397000	1.9095510000

MECP5
Gas phase Energy: -1609.21245499711 hartrees
Solvation Energy: -0.01674169707 hartrees
Zero Point Energy: 340.354 kcal/mol
Free Energy: -37.168 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.2346388151	-0.0892269314	0.1885666083
C2	0.1137808700	0.0466570400	3.7501479000
C3	2.3287533300	0.0378090700	2.6900611500
C4	1.9725734000	-1.2831714800	1.9832881400
N5	0.5158100400	-1.5210894900	1.8132510400
C6	-0.2437015000	-1.3023988500	3.0805246400
C7	-1.7443203700	-1.5152236600	2.8365717500
C8	-2.0240921900	-2.9312091200	2.3100053000
C9	-1.1628491400	-3.2288618700	1.0744199500
C10	0.3104059700	-2.9163695800	1.3411201200
C11	1.6178080700	0.0595636800	4.0516829900
C12	-0.2396930400	1.3364247800	2.9806935500
N13	0.5364947922	1.5087715985	1.7297282155
C14	2.0120107200	1.3231372000	1.8874879200
C15	2.7289087000	2.5569450000	2.4882762600
C16	0.8673243400	4.0322071100	1.6643183400
C17	2.3885702300	3.8472819100	1.7291069500
C18	0.2174302800	2.7890755900	1.0406784200

H19	-0.4572840100	0.0787463100	4.6868269200
H20	3.4166237200	0.0198413700	2.8330513300
H21	2.4272452600	-1.3266272700	0.9884851200
H22	2.4087251200	-2.1043967300	2.5816836900
H23	0.0827007800	-2.0798843300	3.8000879100
H24	-2.2817473400	-1.3421643000	3.7773908800
H25	-2.0996182000	-0.7759109500	2.1077223900
H26	-1.7987894300	-3.6611433200	3.1006631700
H27	-3.0871967700	-3.0451132500	2.0703876100
H28	-1.2500109500	-4.2837034200	0.7874441200
H29	-1.5035067600	-2.6290305900	0.2224925700
H30	0.9013410000	-3.0479296800	0.4298616600
H31	0.7103832400	-3.6120686100	2.1025399900
H32	1.8916423100	0.9418619800	4.6393019000
H33	1.9030095700	-0.8193870100	4.6432659100
H34	-0.0817769900	2.1788523100	3.6753783500
H35	-1.2975323600	1.3490858000	2.7021292800
H36	2.3937577300	1.1934199200	0.8652940900
H37	3.8098460200	2.3707402400	2.4657969500
H38	2.4577260700	2.6840703500	3.5436529100
H39	0.6028279700	4.9077010600	1.0597462800
H40	0.4693355000	4.2159901900	2.6714214700
H41	2.7898540500	3.7894234200	0.7071836000
H42	2.8698309800	4.7075776400	2.2081014300
H43	-0.8722101800	2.8784014000	1.0031394000
H44	0.5589094300	2.6881049500	0.0042486400
H45	-4.3101987143	1.4140244277	-0.2499635246
Cl46	-3.8578956292	1.8633083152	1.4587016594
N47	-4.7088367601	1.1900698907	-1.2568086661
C48	-4.5032955412	-0.2613309080	-1.5131765726
C49	-6.1500276483	1.5442969934	-1.1867202677
C50	-3.9622593464	2.0411741872	-2.2251178747
H51	-3.4333040160	-0.4680610488	-1.5696063908
H52	-4.9474163206	-0.8214350570	-0.6883798781
H53	-4.9863514490	-0.5363956467	-2.4554874889
H54	-6.6244551686	0.9331757295	-0.4175838017
H55	-6.2377429190	2.5943487594	-0.9048358148
H56	-6.6244567422	1.3692401910	-2.1564160407
H57	-2.9035590684	1.7803147718	-2.1648763997
H58	-4.3433006948	1.8668922411	-3.2355378964
H59	-4.1042264089	3.0860122940	-1.9460561099
O60	-1.1342031894	-0.6418771733	-1.7472966667
O61	-1.0638242378	0.6739539062	-1.6077520071

MECP8
Gas phase Energy: -1434.72662813227 hartrees

Solvation Energy: -0.01100196001 hartrees
Zero Point Energy: 263.946 kcal/mol
Free Energy: -29.783 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.2576282200	-0.0157558200	0.1668498200
C2	0.1239544000	0.0517332800	3.7537144200
C3	2.2957505900	0.0313306300	2.6121910700
C4	1.9034661800	-1.2802444900	1.9061606300
N5	0.4359165000	-1.4995070800	1.7820074600
C6	-0.2721537000	-1.2816806400	3.0827655400
C7	-1.7820738100	-1.4852584600	2.9105936700
C8	-2.0847672000	-2.9118031400	2.4313306200
C9	-1.2915495500	-3.2220624100	1.1564358500
C10	0.1956272700	-2.8959565200	1.3149080100
C11	1.6373397500	0.0448803400	4.0003822000
C12	-0.2534736400	1.3471793500	3.0112339500
N13	0.4803870200	1.5466673100	1.7336779000
C14	1.9659451200	1.3351112400	1.8427082800
C15	2.7225509600	2.5398654600	2.4563262200
C16	0.8542383000	4.0716401800	1.7981947400
C17	2.3722657000	3.8671662300	1.7730734400
C18	0.1621396100	2.8783562500	1.1314775700
H19	-0.4121881000	0.0769496000	4.7110345400
H20	3.3877882100	0.0010796200	2.7144520600
H21	2.3288294500	-1.3284891500	0.8987503400
H22	2.3426102200	-2.1105600600	2.4874763900
H23	0.0809145700	-2.0701332300	3.7752273800
H24	-2.2725987000	-1.2882473700	3.8719987900
H25	-2.1728685000	-0.7586727600	2.1866966800
H26	-1.8123043000	-3.6226924300	3.2243442500
H27	-3.1582533800	-3.0363802300	2.2521484200
H28	-1.3813060400	-4.2814958500	0.8894306100
H29	-1.6899052700	-2.6492563000	0.3139772900
H30	0.7085421600	-3.0173640400	0.3578396200
H31	0.6570254400	-3.5861279500	2.0436066400
H32	1.9438299900	0.9149161200	4.5890452800
H33	1.9329062000	-0.8440044000	4.5712677900
H34	-0.0680201600	2.1825200500	3.7041615800
H35	-1.3205648500	1.3690302500	2.7706383700
H36	2.3136639000	1.2277772500	0.8064286700
H37	3.7976316100	2.3362280200	2.3781159600
H38	2.5027691300	2.6267925000	3.5270627900
H39	0.5696555300	4.9778158100	1.2513523700
H40	0.5092818900	4.2120341000	2.8314595800

H41	2.7183189000	3.8507130200	0.7302810200
H42	2.8936551700	4.6954020400	2.2661734000
H43	-0.9253810600	2.9825088300	1.1340762000
H44	0.4573711000	2.8332214600	0.0805488600
O45	-0.3852086200	-1.5607312100	-1.2697592000
O46	-0.6539002100	-1.2348825300	-2.5695023400
H47	-0.9310080100	-0.2729527600	-2.5119940700
Cl48	-1.2028932800	1.5189226300	-1.5779568100

MECP12
Gas phase Energy: -973.88242596553 hartrees
Solvation Energy: -0.00868767835 hartrees
Zero Point Energy: 255.225 kcal/mol
Free Energy: -30.132 kcal/mol
final geometry:

angstroms

atom	x	y	z
Pd1	-0.2346387700	-0.0892269800	0.1885665600
C2	0.1137808700	0.0466570400	3.7501479000
C3	2.3287533300	0.0378090700	2.6900611500
C4	1.9725734000	-1.2831714800	1.9832881400
N5	0.5158100400	-1.5210894900	1.8132510400
C6	-0.2437015000	-1.3023988500	3.0805246400
C7	-1.7443203700	-1.5152236600	2.8365717500
C8	-2.0240921900	-2.9312091200	2.3100053000
C9	-1.1628491400	-3.2288618700	1.0744199500
C10	0.3104059700	-2.9163695800	1.3411201200
C11	1.6178080700	0.0595636800	4.0516829900
C12	-0.2396930400	1.3364247800	2.9806935500
N13	0.5364947600	1.5087716000	1.7297282300
C14	2.0120107200	1.3231372000	1.8874879200
C15	2.7289087000	2.5569450000	2.4882762600
C16	0.8673243400	4.0322071100	1.6643183400
C17	2.3885702300	3.8472819100	1.7291069500
C18	0.2174302800	2.7890755900	1.0406784200
H19	-0.4572840100	0.0787463100	4.6868269200
H20	3.4166237200	0.0198413700	2.8330513300
H21	2.4272452600	-1.3266272700	0.9884851200
H22	2.4087251200	-2.1043967300	2.5816836900
H23	0.0827007800	-2.0798843300	3.8000879100
H24	-2.2817473400	-1.3421643000	3.7773908800
H25	-2.0996182000	-0.7759109500	2.1077223900
H26	-1.7987894300	-3.6611433200	3.1006631700
H27	-3.0871967700	-3.0451132500	2.0703876100
H28	-1.2500109500	-4.2837034200	0.7874441200
H29	-1.5035067600	-2.6290305900	0.2224925700

H30	0.9013410000	-3.0479296800	0.4298616600
H31	0.7103832400	-3.6120686100	2.1025399900
H32	1.8916423100	0.9418619800	4.6393019000
H33	1.9030095700	-0.8193870100	4.6432659100
H34	-0.0817769900	2.1788523100	3.6753783500
H35	-1.2975323600	1.3490858000	2.7021292800
H36	2.3937577300	1.1934199200	0.8652940900
H37	3.8098460200	2.3707402400	2.4657969500
H38	2.4577260700	2.6840703500	3.5436529100
H39	0.6028279700	4.9077010600	1.0597462800
H40	0.4693355000	4.2159901900	2.6714214700
H41	2.7898540500	3.7894234200	0.7071836000
H42	2.8698309800	4.7075776400	2.2081014300
H43	-0.8722101800	2.8784014000	1.0031394000
H44	0.5589094300	2.6881049500	0.0042486400
O45	-1.1342032100	-0.6418772300	-1.7472965800
O46	-1.0638242300	0.6739540100	-1.6077520600

O_2
Gas phase Energy: -150.31662272463 hartrees
Solvation Energy: -0.00000001966 hartrees
Zero Point Energy: 2.376 kcal/mol
Free Energy: -12.537 kcal/mol
final geometry:

angstroms

atom	x	y	z
O1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	1.2140596102

H_2O_2
Gas phase Energy: -151.54014695781 hartrees
Solvation Energy: -0.00738548798 hartrees
Zero Point Energy: 16.536 kcal/mol
Free Energy: -13.625 kcal/mol
final geometry:

angstroms

atom	x	y	z
O1	-0.0322135748	-0.7272903172	0.0292595249
O2	0.0322135748	0.7272903172	0.0292595249
H3	0.7786519618	-0.9275659694	-0.4643698940
H4	-0.7786519618	0.9275659694	-0.4643698940

$N(CH_3)_3$
Gas phase Energy: -174.48281581527 hartrees
Solvation Energy: -0.00190507992 hartrees
Zero Point Energy: 75.682 kcal/mol

Free Energy: -17.121 kcal/mol
final geometry:

angstroms

atom	x	y	z
N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4549019751
C3	1.3527449496	0.0000000000	-0.5358376672
C4	-0.7884115347	-1.0991140594	-0.5359029551
H5	0.5481981761	0.8723436199	1.8260071561
H6	-1.0282944139	0.0636883554	1.8261311850
H7	0.4644962979	-0.9054707799	1.8948000024
H8	1.9329467062	-0.9052008532	-0.2654612675
H9	1.3191002850	0.0628401406	-1.6286330563
H10	1.8995309702	0.8727491019	-0.1635938678
H11	-0.3908202316	-2.0982928775	-0.2661681479
H12	-1.8160530544	-1.0351404216	-0.1629037671
H13	-0.8206030556	-1.0345312278	-1.6286282054

$HN(CH_3)_3$•Cl
Gas phase Energy: -635.31125605755 hartrees
Solvation Energy: -0.01814799244 hartrees
Zero Point Energy: 83.437 kcal/mol
Free Energy: -20.119 kcal/mol
final geometry:

angstroms

atom	x	y	z
N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4821600104
C3	1.3700615671	0.0000000000	-0.5651261387
C4	-0.8446135919	-1.0787951121	-0.5654512069
H5	0.4517057137	-0.9204102256	1.8655267984
H6	0.5619965950	0.8672007316	1.8319037220
H7	-1.0298277236	0.0855039111	1.8318630466
H8	1.8932088393	-0.9248543464	-0.3022645604
H9	1.3007857651	0.0962020949	-1.6496474243
H10	1.9111684222	0.8613751649	-0.1709060118
H11	-0.4441871787	-2.0609715358	-0.2951121948
H12	-1.8586862399	-0.9678172383	-0.1786780144
H13	-0.8702597029	-0.9701890153	-1.6507191942
H14	-0.4887721667	1.0021191826	-0.3279515145
Cl15	-1.2034840099	2.4657426458	-0.8103503431

$HN(CH_3)_3^+$
Gas phase Energy: -174.86272209860 hartrees
Solvation Energy: -0.05957781653 hartrees
Zero Point Energy: 85.538 kcal/mol

Free Energy: -17.316 kcal/mol
final geometry:

angstroms

atom	x	y	z
N1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.5070847502
C3	1.3999438417	0.0000000000	-0.5584709695
C4	-0.8243474806	-1.1311200861	-0.5594040663
H5	0.5618184825	0.8651631621	1.8601709639
H6	-1.0302795714	0.0507735673	1.8600499755
H7	0.4709510003	-0.9210258972	1.8528466851
H8	1.8935889486	-0.9233176899	-0.2526662945
H9	1.3459359726	0.0554545857	-1.6459741370
H10	1.9370449035	0.8625958368	-0.1635072294
H11	-0.3700136735	-2.0740125061	-0.2524187723
H12	-1.8385627624	-1.0564035716	-0.1664614980
H13	-0.8352709983	-1.0551873073	-1.6470246804
H14	-0.4441918606	0.8737121061	-0.3012233210

HCl
Gas phase Energy: -460.80006383205 hartrees
Solvation Energy: -0.00318039114 hartrees
Zero Point Energy: 4.238 kcal/mol
Free Energy: -11.224 kcal/mol
final geometry:

angstroms

atom	x	y	z
Cl1	0.0000000000	0.0000000000	0.0000000000
H2	0.0000000000	0.0000000000	1.2854696004

Ket
Gas phase Energy: -193.16058936631 hartrees
Solvation Energy: -0.00458646313 hartrees
Zero Point Energy: 52.601 kcal/mol
Free Energy: -17.204 kcal/mol
final geometry:

angstroms

atom	x	y	z
O1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.2158363148
C3	1.2933640472	0.0000000000	2.0145208581
C4	-1.2933651703	0.0000229499	2.0145199099
H5	2.1466343615	0.0000046165	1.3348718676
H6	1.3416082105	0.8802456599	2.6664000210
H7	1.3416135366	-0.8802249585	2.6664286247
H8	-2.1466429578	0.0001426098	1.3348785640

H9	-1.3416582658	-0.8802646497	2.6663461693
H10	-1.3415367416	0.8802100437	2.6664880844

Tol
Gas phase Energy: -271.57264040502 hartrees
Solvation Energy: -0.00205382317 hartrees
Zero Point Energy: 80.377 kcal/mol
Free Energy: -18.156 kcal/mol
final geometry:

angstroms

atom	x	y	z
C1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4031688971
C3	1.3005357347	0.0000000000	-0.7690885751
C4	-1.1949520638	-0.0004927465	2.1212772405
C5	-2.4189869548	-0.0009443365	1.4474063715
C6	-2.4338755484	-0.0008773909	0.0529338055
C7	-1.2336207133	-0.0003932274	-0.6617124671
H8	1.9051606829	-0.8832274799	-0.5321648841
H9	1.1263260732	0.0040057300	-1.8486730732
H10	1.9089246720	0.8789248047	-0.5260176440
H11	0.9478112711	0.0003386231	1.9366974540
H12	-1.1717556255	-0.0004897052	3.2077182728
H13	-3.3507674437	-0.0012923666	2.0053531595
H14	-3.3792904146	-0.0011571935	-0.4822859403
H15	-1.2547921047	-0.0003313959	-1.7487863714

Spar
Gas phase Energy: -696.77937555249 hartrees
Solvation Energy: -0.00078063987 hartrees
Zero Point Energy: 250.622 kcal/mol
Free Energy: -24.739 kcal/mol
final geometry:

angstroms

atom	x	y	z
H1	0.5896412934	2.6206082340	0.1257213878
C2	0.1006195190	-0.0894310256	3.7385344534
C3	2.3297790861	-0.0773121633	2.7016487868
C4	1.9505548453	-1.3341489308	1.9003325478
N5	0.5129672989	-1.4837700163	1.6900161417
C6	-0.2956195052	-1.3388675833	2.9106633405
C7	-1.7889891785	-1.3666600898	2.5464009220
C8	-2.1592835871	-2.6494455912	1.7911735136
C9	-1.2506846364	-2.8121564862	0.5671588976
C10	0.2213143585	-2.7258151396	0.9784620855
C11	1.6012009130	-0.1430731767	4.0518335621

C12	-0.1984259726	1.2774418220	3.0937558055
N13	0.5737403149	1.4941745282	1.8752092727
C14	2.0222905640	1.2498859944	1.9675496159
C15	2.7954217214	2.4484531966	2.5755117910
C16	0.9547503431	3.9823705918	1.7614541385
C17	2.4723570632	3.7537991090	1.8292250521
C18	0.2666152912	2.7362150657	1.1718935640
H19	-0.4779231202	-0.1387286837	4.6707499396
H20	3.4157819646	-0.1165530992	2.8581464862
H21	2.4333765804	-1.3118015346	0.9143267925
H22	2.3749248714	-2.2111623235	2.4371242289
H23	-0.1100770969	-2.2075518831	3.5850594925
H24	-2.3851707213	-1.2712602892	3.4628995912
H25	-2.0147448273	-0.5007602561	1.9134697236
H26	-2.0336501717	-3.5156218282	2.4565152821
H27	-3.2146840343	-2.6317388912	1.4942792987
H28	-1.4357833326	-3.7696207930	0.0654413913
H29	-1.4620220456	-2.0161608528	-0.1575608639
H30	0.8621110073	-2.7663355530	0.0891582585
H31	0.4807330277	-3.6147028240	1.5952037319
H32	1.8890220203	0.6846338086	4.7103363820
H33	1.8595637147	-1.0731588244	4.5740950364
H34	-0.0225498512	2.0439334846	3.8767097914
H35	-1.2599776327	1.3566908141	2.8303315111
H36	2.3757581942	1.1423357939	0.9286673753
H37	3.8737268246	2.2458113730	2.5374401936
H38	2.5363061276	2.5651555267	3.6359090692
H39	0.7205795770	4.8639428260	1.1514228652
H40	0.5641444464	4.1830817190	2.7682108326
H41	2.9746465267	4.6033601041	2.3072116809
H42	2.8710246999	3.6918467203	0.8057409819
H43	-0.8223692501	2.8637196270	1.1532846709

Spar-H•Cl
Gas phase Energy: -1157.61092341285 hartrees
Solvation Energy: -0.01521962143 hartrees
Zero Point Energy: 260.101 kcal/mol
Free Energy: -26.721 kcal/mol
final geometry:

	angstroms		
atom	x	y	z
H1	0.3027115185	2.4759178669	0.0556753325
C2	-0.0186463703	-0.1149967366	3.6868515397
C3	2.1899360716	-0.0892300116	2.5792245917
C4	1.8173813197	-1.3100083232	1.7261489521
N5	0.3335359051	-1.4436850943	1.5182151440

C6	-0.4815424398	-1.2887406426	2.7922470278
C7	-1.9682695540	-1.2822744999	2.4184714441
C8	-2.3688963114	-2.5907033080	1.7196722080
C9	-1.4748846488	-2.8404806022	0.4979394342
C10	0.0103448017	-2.7571888490	0.8469904617
C11	1.4929105015	-0.2166952440	3.9429937457
C12	-0.3125479660	1.2825921677	3.1210547404
N13	0.3798139204	1.4516696523	1.8531834356
C14	1.8412793127	1.2503982821	1.8843858118
C15	2.5978725832	2.4639221045	2.4697147637
C16	0.7062924205	3.9324626592	1.6291869448
C17	2.2308303123	3.7392050257	1.6891753784
C18	0.0221884743	2.6592619430	1.0995070860
H19	-0.5676105959	-0.2302485073	4.6304246918
H20	3.2789809733	-0.1299562722	2.7053487574
H21	2.2440613186	-1.2483399367	0.7219212846
H22	2.1644381324	-2.2297920486	2.2115646841
H23	-0.2718613794	-2.2082765721	3.3591498041
H24	-2.5534377549	-1.1354671101	3.3336737478
H25	-2.1725573400	-0.4302582784	1.7603491429
H26	-2.2788939740	-3.4241049092	2.4311157093
H27	-3.4198516669	-2.5495784854	1.4151815971
H28	-1.6681477413	-3.8284914376	0.0656929320
H29	-1.6733737041	-2.0986789018	-0.2831894152
H30	0.6185742390	-2.7927191199	-0.0581095538
H31	0.3193576339	-3.5532233525	1.5353450230
H32	1.8099153150	0.5784940454	4.6256041136
H33	1.7535537531	-1.1705532038	4.4204461575
H34	-0.0454050512	2.0223014455	3.9018624549
H35	-1.3852945682	1.4102464506	2.9364798940
H36	2.1379058622	1.1587634127	0.8302187433
H37	3.6796251614	2.2843930351	2.4179019347
H38	2.3522638561	2.5983267157	3.5319545381
H39	0.4535652563	4.7816136711	0.9828035719
H40	0.3257958785	4.1779644732	2.6307495948
H41	2.7165033262	4.6140282525	2.1372467907
H42	2.6208610783	3.6526825585	0.6655023259
H43	-1.0685937931	2.7634988546	1.1164525642
H44	0.1015291468	-0.7023287996	0.7685903466
Cl45	0.2130450553	-0.1305787766	-1.1643782057